İSTANBUL TECHNICAL UNIVERSITY ★ INSTITUTE OF SCIENCE AND TECHNOLOGY

SIMULATION OF RADIANT HEATING SYSTEM USING CFD (FLUENT)

M.Sc. Thesis by
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Programme: Automotive Engineering

Supervisor : Assoc. Prof. Dr. Doğan GÜNEŞ

MAY 2003

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ÖNSÖZ

Eğitimin giderek bilimsellikten uzaklaştığı günümüzde, böyle bir çalışma yapmak heyecan verici. Diğer taraftan zamanın herşeyden fazla değer kazandığı günümüzde, mühendislikte zamandan ve pahadan kazanç sağlayan simülasyon üzerine çalışma yapma fırsatı bulmuş olmamdan ötürü sevinçliyim.

Bu çalışmada benden destek ve yardımlarını esirgemeyen değerli hocam Sayın Doç. Dr. Doğan Güneş'e teşekkürlerimi sunuyorum.

Ayrıca bu çalışmada destek ve yardımlarını gördüğüm Gözde Cömert, Mehmet Tirgil ve Levent Timur'a teşekkürü bir borç bilirim.

Oğuz Kurtili Mayıs 2003

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ÖZET

Günümüzde zamanla yarışmanın ve ekonominin önemi geçmişe göre artmıştır. Bu çalışma, mühendislik çalışmalarında yığınla deney yapmanın ve bu deneylerin yol açtığı mali külfetlerin bir nebze önüne geçen simulasyon çalışmalarına bir örnektir.

Bu çalışmada simülasyonu yapılmak üzere, günümüzde de oldukça geniş bir kullanım alanına sahip olan radyant ısıtma sistemi tercih edilmiştir. Bu sebeple, çalışmanın birinci bölümünde radyant ısıtma sistemleri tanıtılmıştır. Bu amaçla; sistemlerin çalışma prensiplerinden, avantajlarından, dezavantajlarından, diğer sistemlere göre daha fazla seçilme nedenlerinden kısaca bahsedilmiştir.

İkinci bölümde gaz yakıtlar hakkında genel bilgiler verilmiş, sıvı ve gaz yakıtla çalışan ısıtma sistemlere yer verilmiş ve radyant ısıtma sistemlerinin başlıca yakıtı olan dogal gaz ve onun en önemli bilşeni metan gazının özelliklerinden bahsedilmiştir.

Üçüncü bölümde hidrokarbonların yanma mekanizmları ele alınmış, özellikle çalışmanın yapıldığı metan gazı üzerinde durulmuştur.

Dördüncü bölümde ise simulasyon yapmak için kullanılan CFD (Computational Fluid Dynamics) anlatılmış, programın kullandığı korunum denklemlerinden ayrıntıyla bahsedilmiş; simulasyonun getirdiği avantajlar sıralanmıştır. Sonrasında simulasyonu yapılacak deney tesisatı tanıtılmış, simülasyon yaparken izlenmesi gereken adımlar anlatılmıştır.

Dördüncü bölümün sonunda ise sonuçlar değerlendirilmiştir. Bu değerlendirme için, bu deney tesisatı ile daha önce yapılmış bir çalışmanın sonuçlarından faydalanılmıştır. Simülasyon hakkındaki genel görüşlere de bu bölümde yer verilmiştir.

SUMMARY

In this study radiant heating system was simulated by using CFD. Firstly, radiant heating systems that are very common in use nowadays introduced briefly and working principles were dictated. It was mentioned about the combustion mechanism of methane, which is the main component of these systems fuels, while working principles were dictated. Than, CFD was introduced and its advantages were mentioned. The combustion mechanisms used by this software were investigated. Finally, a simulation of a radiant system - this system had been investigated as a license study before - was done by using Fluent 6.0 and the results were compared.

Generally speaking, simulation is used almost in all engineering applications because of its properties such as usefulness, easiness, cheapness and quickness. But its reliability is disputable. To prove the reliability of the simulation many experiments are needed. This study is one of them.

Radiant heating system is referred in order to make simulation in this study, because it is very common in use in heating application both homes and factories. Radiant heating is comfortable, clean and healthful, unobtrusive, energy-efficient, less costly to purchase that are why radiant heating is preferred. First part of the study relates to this.

General knowledge's about gaseous fuels were given in the second part of this study. The properties of the natural gas were mentioned, because natural gas is most common fuel in radiant heating. Liquid and gaseous burners were told briefly as last topic of this section.

Chapter three touches on the combustion mechanism of hydrocarbons. Because of methane is also the main component of natural gas, so its combustion mechanism was investigated in this section.

In order to simulate radiant heating system in this study, CFD was used. CFD's advantages and applications were mentioned in the fourth section of the study. Then, the equations such as mass, momentum, energy conservation those fluent uses were also introduced. The radiant heating test installation was also introduced in this part.

Technical properties of the components were given. Simulation was also done in this section. Some steps that have to be taken to make simulation were defined.

At the last section of chapter four, results of the simulation were compared to results of the tests that had already done before with the same system, and some suggestions were given.

1. RADIANT HEATING SYSTEMS

1.1. Introduction

The necessity for supplying heat in some form to promote human comfort as required by climatic conditions in many parts of the inhabited world is well known, although the factors involved in providing comfort conditions are not always fully understood. With advancing civilization the desire for increase comfort, as well as cleanliness, sanitation, freedom from disease, freedom from petty and repetitive duties, becomes increasingly important, with the result that living conditions, as evidenced in housing design and construction, are continually being improved to meet popular demand.

One of the desired improvements in living conditions has to do with the method of supplying heat to or removing heat from inclosed spaces occupied by human beings in order to produce conditions of maximum comfort. To consider this problem in detail, it will be necessary first to consider one by one all the factors entering into the problem.

The question immediately arises: What is comfort? The expressions often used are ‘’feeling hot’’, ‘’feeling cold’’, or ‘’ feeling comfortable’’, without the clear understanding of the elements that are involved in these simple statements. To visualize these states, it must be realized first that the human body is a self-repairing heat engine, capable of performing work, and as such it is directly comparable in many ways to an internal combustion engine, such as in automobiles. Engines of this type take in air and fuel, convert them into heat energy, deliver some of this energy as work, and reject the remainder, either through radiation and convection from the engine itself or by convection air currents through the radiator and by discarding some of the heat through the exhaust gases. If the engine is deprived of air or fuel or allowed to overheat, operation ceases.

The human being, as with all warm-blooded animals, functions in exactly the same manner. In order to perform work, the animal must be alive and active. To be so, it must draw in air and fuel as represented by food and convert these quantities into energy whereby to repair and maintain the organism and be ready to perform work as

required. The minimum normal heat developed by a human being approximates 500 Btu per hr. (A Btu is a measure of heat and is an abbreviation of British thermal unit, which is defined as the amount of heat required to raise the temperature of 1 lb of water 1°F) Of this amount, 100 Btu are used up in maintaining the body in operation and making repairs. The remaining 400 Btu have to be dissipated; otherwise, the body would overheat and trouble would develop exactly as with an internal combustion engine. 190 Btu of this may occur by radiation, 110 Btu per hr by convection and evaporation and 100 Btu per hr by exhalation.

The body has other methods of disposing of heat, but these are of negligible importance. With heat being dissipated at the previously mentioned rate and in the proportions indicated, the temperature of the body would remain normal at 98.6 °F.

Assume now that a subject is exposed to an environment of normal conditions, such as 70 °F air temperature, 50 percent relative humidity, no direct radiant heat, no air currents, and that the subject is suitably clothed. Assume further that the Btu radiated, dissipated, and lost by convection, evaporation, etc., are in accordance with the preceding table. Under this conditions it can be assumed that the subject is comfortable. In other words, he has no sensation of either heat or cold.

Now assume that the environment changes so that it is no longer possible with the amount of Btu radiated to continue at 190 Btu per hr. Than with other conditions remaining the same, the temperature of the body will tend to go up because as the body is continuing to generate heat, and if the flow of heat away from the body is impeded, the temperature of the body must go up. The nerves on the surface of the skin will note this tendency, which is one of the body's methods of sensing its environment. Other methods are, of course, through the eyes and ears. The tendency toward a temperature increase is reported to that section of the brain believed to be in the area of the thalamus, which is presumed to be center of the temperature control. Following receipt by the brain of the tendency to temperature increase, the nerve center makes the necessary corrective efforts: first, it causes the blood vessels leading to the surface of the body to expand, thereby increasing the loss of heat by greater blood circulation; then it may increase the rate of breathing so that the loss by exhalation will be increased; and lastly, it may stimulate the sweat glands in order to increase the losses by evaporation. These corrections are all made automatically, without conscious effort on the part of the subject, and have been caused by the sensation of feeling warm.

Consider now the chain of events that takes place should be environment change from the previous comfort condition of 70° temperature, 50 percent humidity, no

direct radiation or air currents, and assume that radiation and other losses increase by reason of lower external temperatures or for other causes. The rate of heat loss from the body will increase, and the fall in temperature will be noted by the nerves of the skin, with the result that the thermal center of the brain takes cognizance of the fact that the heat losses above normal, thus automatically setting up suitable corrective measures, such as reducing heart action, thus reducing flow of the blood to the surface of the body, and thereby directly reducing the loss by radiation and convection. In order to assist further in the reduction of loss of heat by the flow of blood to the surface of the body, the blood vessels are contacted so as to decrease the supply of blood to the skin and body surface. By these means and concomitant measures, proper body temperature is maintained.

If these corrective factors are insufficient to compensate for excessive loss, then the body resorts to the phenomenon known as shivering, which is merely using up muscular energy, and by doing so produces heat, attempting in this way to maintain heat balance by generating more heat to counteract excessive loss.

If all the above described normal corrective measures available to the nervous system of the body are insufficient to maintain proper body temperature, then further corrective measures for the protection of life are obtained by the nervous system by accentuating the feeling of discomfort to such an extent the individual concerned takes the necessary steps to adjust or modify the environment so that bodily heat loss will be reestablished to normal values. Such steps would include putting on more clothing, building a fire, etc.

The human machine is not so efficient. If it is producing work at the rate represented by 115 net Btu per hr, which can be regarded as a measure of reasonable maximum activity on the part of a man, than the total Btu that have to be dissipated amount to approximately 1300 per hr. As a result, although radiation does increase, most of the heat loss must be dissipated through convection, evaporation, and exhalation. Consequently, when a human being is performing heavy work, he must be provided with an environment that will allow the dissipation or absorption of a relatively large bodily Btu output. This is the reason why rooms occupied by people engaged in heavy manual work must be maintained at lower average temperatures than room occupied solely by mental workers.

Radiant heating and cooling are directed toward the control of comfort by influencing by radiant component of bodily heat output rather than by adjusting the convection and evaporative elements to secure bodily heat balance as is methods used by conventional systems; hence, radiant heating is not simply another type of

heating but is a distinctly different method of providing comfort from any or all of the presently known conventional methods.

If the preceding discussion is reduced to the simplest terms, it can be observed that in a conventional system the determining factor for comfort in the enclosure to be heated is the air temperature in this enclosure. In a radiant heating system, comfort can be had independently of the air temperature. This is not true of any other method of heating.[1,5]

1.2. Definition Of Radiant Heating

There are three ways to heat transfer among the materials: Conduction, convection and radiation. In conduction, there may be only one solid or connected multiple solids. In convection there are two connected substances, one is solid and other is fluid.

Heat transfer by radiation is different in many ways than others. Heat radiation is a kind of electromagnetic radiation. Heat radiation can be defined as electromagnetic transfer between two surfaces. Convection heat transfer occurs through air. There is no need such a tool in heat radiation. Objects, masses and surfaces is heated by heat radiation; not directly air.[1,2,5]

1.3. What Is Radiant Heating

Radiant heating systems can be defined as they are the systems that spread more than half of its energy by infrared radiation. This means the systems surfaces are over 100°C in practice. There are gas fuel radiant pipes, plaques, electric quartz heaters and radiant panels among radiant heating systems. Human being perceive the heat radiation by two ways at radiant heating system environment:

1. Directly from heat source
2. Indirectly from walls and floor. If the walls are good isolated, sense of warm increase as close to wall.

Radiant heating systems can be divided into two parts depending on surface temperatures.

There are many kind of radiant system of this systems: High and middle density systems, and low-density systems. If the surface temperature is over 815°C, it is known as high temperature radiant heating; if it is less than 815°C then it is known as low-temperature systems.

The radiant system that was used in experiment and simulation is also low-temperature radiant system. These kinds of systems are preferred much more than others in application. These systems have a pipe that's outer surface diffusion properties are increased. A burner gives fuel into this pipe with a fan. Than fuel is burned. Radiation occurs as increase the heat of the pipe surface. Exhaust gases are vacuumed by a vacuum pump.[2]

1.4. Reasons For Choosing Radiant Heating

There are two main reasons:

1. Less heating expends than the other systems
2. Providing heating the places that are not heated by the other systems.

The preference reasons could be well understood when radiant heating and conventional heating are compared. Fallowing table compares this two.

Table 1.1. Comparing radiant heating systems and conventional heating systems

Advantages of radiant heating	Disadvantages of radiant heating
▪ High efficiency, less heat input ▪ Short preheating time, regulating opportunities according to conditions ▪ Increase heating comfort in hard heated spaces ▪ Don't take place on the useful ground ▪ Don't pollution	▪ Repairing expends depends on montage high ▪ Shade effects that may cause to increase radiation ▪ More than needle heating at close to burner ▪ High temperature necessity in some buildings

Low operating cost and energy efficiency of the system are the reasons of choosing radiant heating systems in many situations. Although low energy input than other system, it supplies comfortable environment. In conventional systems heat is transferred to air than spread to building by convection. But in radiant heating heat is transferred to the walls and floor of the building, than spread to air by convection. More than half of the heat loss in big buildings occurs due to air losses. These losses depend on the difference between internal and external air temperature. If the same heating comfort could were provided by decreasing 3°C of internal air temperature, air leak loss could be decreased % 30 through the heating season.[5]

1.5. Alternatives Of Radiant Heating Systems

Radiant heating systems are defined as the systems that's spreading heat is over 100°C practically. General radiant heating systems are shown in the following table.

Table 1.2- General classification of radiant heating systems

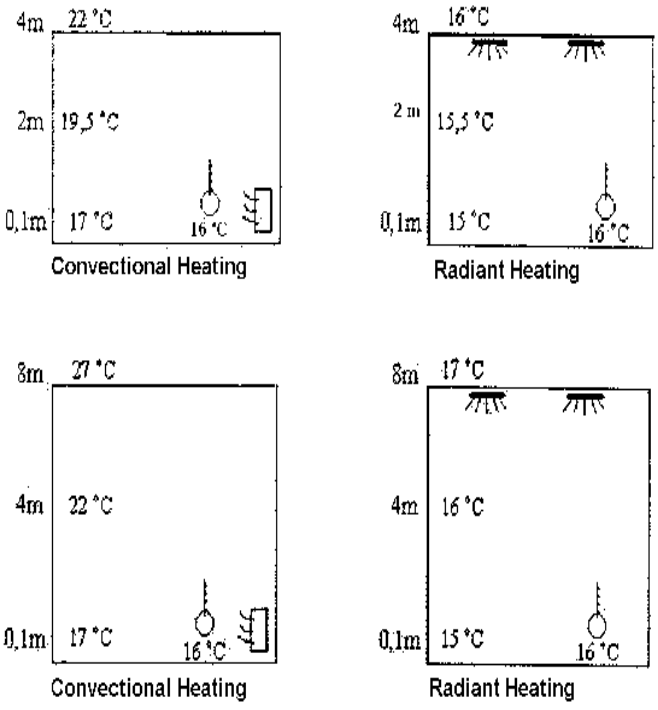
Fuel	**Heat transfer fluid**	**System type**	**Temperature of spreader**
Solid Fuel	Water at average or high temperature	Hot water pipes or panels	100 – 150 °C
	Steam	Steam pipes or panels	100 – 180 °C
Gas or Fuel Oil	Air	Air heating radiant pipe	100 – 150 °C
Gas	Hot gases	Gas burner radiant pipe	200 – 500 °C
	None	Plaques and cones	800 – 900 °C
Electricity	None	Resistance	1000 °C
	None	Linear quartz tube	2000 °C

1.6. Advantages Of Radiant Heating Systems

1- Heat loss is prevented at high spaces.

2- The radiant heater does not take up useful space. This is true in the first place for heaters built in the border structures, which are not even visible. But the statement goes for radiant panels, too, as they are mostly placed under the ceiling and thus do not interfere with the equipment in the room.

3- Radiant heating surfaces can be turned in summer into cooling surfaces with an appropriate cooling medium.



4- Convection heating causes dust deposit in the structures; this cannot happen with radiant heating.

5- In certain cases, when only parts of the space need to be heated, the installation cost is smaller than that of traditional convection heaters.[1,5]

1.7. Radiant Pipe Heating Systems Operating On Gas

Gaseous fuel radiant heating systems can be defined as a burner connected to a steal pipe. Generally there is a vacuum pump for burned gas. Radiant systems form from pipes those can be straight, U type, or many pipes connected to each other. It is possible that 10-40 kW heat generation can be obtained by the one-unity systems with U pipe type. 180 kW heat can be obtained by multiple pipe heating systems. The table below shows the advantages and disadvantages of the one unity radiant pipe heating systems.

Table 1.3. Advantages and disadvantages of radiant heating systems

Advantages	Disadvantages
• Low weight • Flexible installation and uninstallation • The time to be on is low • Low investment cost • If there is enough fresh air inlet, some of the exhaust gas could be let inside • If there is insufficient temperature, desired conditions can be supplied with one or more pipes.	• Limited fuel alternatives (in general, natural gas or LPG) • The exhaust gases which is given to the environment increase the ratio of humidity and CO_2 • It is not suitable some environments that includes substance those have oxidation, toxide effects • Radiant efficiency reduce due to bending the pipes while fitting to the wall • Works little noisy cause of exhaust fan

The plate on the steal pipe loses its future by time. Some of the producers make noncorrosive steal pipe for burning part of the pipe, low quality steal is used for the other parts of the system. The spiral gas reflectors that is put into radiant pipe, are used to make turbulence and increase the heat transfer from burned gas to the in face of the pipe.

Radiant pipe is fixed to the reflector, which is made of aluminum or noncorresive steal. Using isolationed reflectors provides increasing on efficiency, but they are not used too much. The figure at the bottom illustrates a radiant heater.

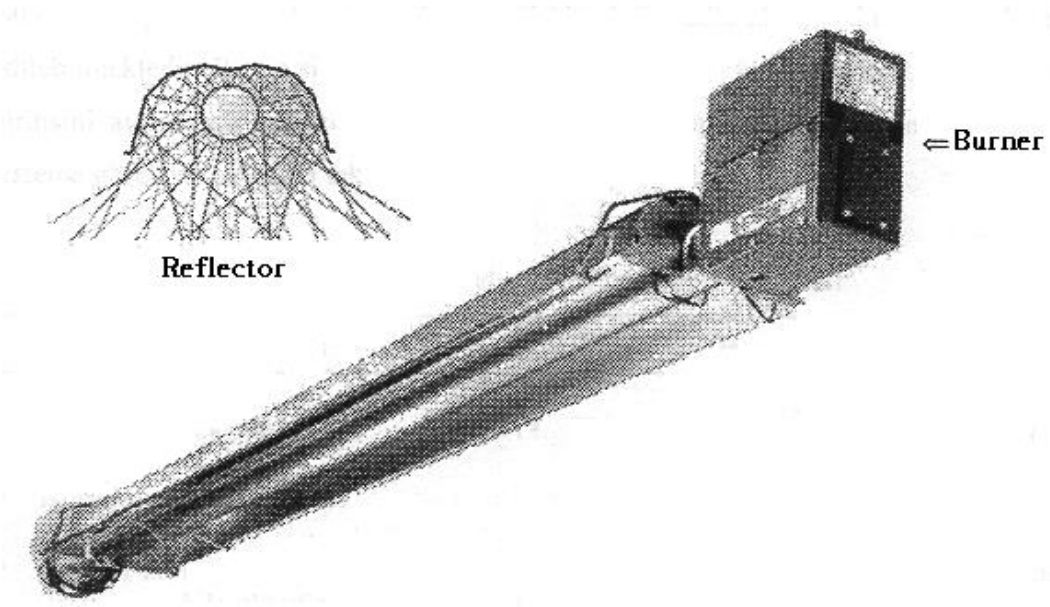


Figure 1.1. Radiant Heater

Isolation of reflectors and plaques reduce the conduction heat loss and increase efficiency of radiant heating.

Single and U type pipes can be bend on the pipe axis in order to fit the system to the wall. This causes to an increase on the heat loss with conduction. Most producers

suggest ±15° maximum angles for normal radiant heating applications. This angle could increase to 55° in applications of fitting to wall.

Continual radiant pipe systems are made up of an exhaust fan and a long pipe that has various burners. Advantages and disadvantages of the continual radiant heating systems are given in the following table.

Table 1.4. Continual radiant heating systems operating on gas

Advantages	Disadvantages
• Quite low weight • Quite good diffusion of radiation • Requiring heat is set by regulation mechanism • Geometry could be chosen • The exhaust fan could be out of the heating environment in order to decrease noise	• Relatively less flexible than single unity radiant pipe system • It is not suitable some environments that includes substance those have oxidation, toxide effects • More expensive than single unity radiant pipe system

Radiant heating systems that are used for heating large places such as factory or atelier, generally is made up of multiple-connected pipes, burners that are placed to different parts of the pipes and reflectors that are set on different regions of the pipes. System works be hung to ceiling. Natural gas or LPG is used as fuel. Burnt gases are blow out by exhaust fan. The heat is directed to the human and bodies by the reflectors over the pipes. With this way, human being is warmed up by radiation. Gas fuel-low density radiant heating systems provide clear, homogenous and silent heat because, there is no air blowing process that causes to form dust and different pollutants and lukewarm and cold points. [2]

2. GASEOUS FUELS

2.1. Introduction

Obviously, all gases can be liquefied since every pure compound, depending on temperature and pressure, can exist as s gas, a liquid and/or a vapor. Many gases, in fact, can be condensed simply by compression. Some, such as liquefied natural gas (LNG) and liquid hydrogen, require super cold, or cryogenic, state in order to exist and will not remain in this condition without extreme refrigeration and isolation. For the sake of this discussion, therefore a fuel will be considered to be a gas if it is noncondensable over normal temperatures and pressures. Examples of gaseous fuels include hydrogen gas, methane, and natural and synthetic gas (SNG). Vapors such as propane, butane, and liquefied petroleum gas (LPG) are fuels that are condensable over normal temperatures and pressures. Organizations such as the American Gas Association (AGA) are involved in many aspects of fuel gas technology, including supporting research and development within the natural gas industry, producing synthetic gas via coal gasification, and developing biomass-generated methane systems. Gaseous fuel science will continue to play an important role in combustion engineering in part because of the clean-burning nature of this energy resources, the fact that most fuels actually burn in the gas phase, and insights into the complex nature of general combustion processes being provided by studies of simple gas phase molecular reactions.[3,7]

2.2. Gaseous Fuel Properties

The specific gravity (SG) of gases and liquids is equal to the ratio of density for a particular fluid of interest to that of a reference compound. For liquids, the reference is water; for gases, however, the reference is air. Liquid density is only a function of temperature but, for a gas, density is a function of both temperature and pressure and, therefore, the specific gravity is given as

$$SG_{\text{gas}} = \frac{\rho_{fuel} < 1atm 15.56°C (60°F) >}{\rho_{air} < 1atm 15.56°C (60°F) >} \tag{2.1}$$

If the ideal gas behavior is assumed, the molar density $\overline{\rho}$ of fuel gases is then equal to

$$\overline{\rho} = \frac{P}{\overline{R}T} \frac{kgmole}{m^3} \left(\frac{lbmole}{ft^3} \right) \tag{2.2}$$

and the specific gravity of these fuels is, therefore, equal to

$$SGgas = \left[\left(\frac{MW}{\overline{R}} \right) \left(\frac{P}{T} \right) \right]_{gas} \left[\left(\frac{MW}{\overline{R}} \right) \left(\frac{P}{T} \right) \right]_{air} = \frac{MW_{gas}}{MW_{air}} \tag{2.3}$$

Equation (2.3) shows that a gaseous fuel having a specific gravity of less than 1.0 is lighter than air whereas a fuel having a specific gravity greater than 1.0 is heavier than air. This can be an important factor in gas leakage and safety requirements for storing and handling gaseous fuels. Table 2.1 lists specific gravities and critical constants for several gaseous fuels.

Table 2.1. Gaseous Fuel Specific Gravities

		Critical constants		
			T	
	SG	*P*, atm	°C	(°F)
Paraffins				
Methane	0.554	45.8	−81.9	−116
Ethane	1.049	48.2	32.5	90
Propane	1.562	42.0	97.0	206
Butane (iso)	2.066	36.0	135.3	275
Butane (N)	2.066	37.5	152.6	306
Pentane (nee) 2.2-dimethyl propane	2.487	31.6	160.9	321
Pentane (iso) 2-methylbutane	2.487	32.9	188.1	370
Pentane (N)	2.487	33.3	197.0	386
Hexane (nee) 2.2-dimethylbutane	2.973	30.7	216.4	421
Hexane 2.3-dimethylbutane	2.973	30.9	227.6	441
Hexane (iso) 2-methylpentane	2.973	29.9	225.3	437
Hexane 3-methylpentane	2.973	30.8	231.4	448
Hexane (N)	2.973	−29.9	234.8	454
Heptane 2.2.3-dimethylbutane	3.459	−29.7	258.7	497
Heptane (iso) 2-methylhexane	3.459	27.2	258.1	496
Heptane (N)	3.459	27.0	267.6	513
Octane (iso) 2.2.4-trimethylpentane[a]	3.944	25.5	271.4	520
Octane 2.5-dimethylhexane	3.944	25.0	279.2	534
Octane (N)	3.944	24.6	296.4	565
Nonane (N)	4.428	22.5	322.0	611
Decane (N)	4.915	20.8	345.9	654
Naphthenes				
Cyclopropane	1.451	—	—	—
Cyclobutane	1.938	—	—	—
Cyclopentane	2.422	—	—	—
Cyclohexane	2.905	40.4	281.4	538

Table 2.1. Continued

		Critical constants		
			T	
	SG	P, atm	°C	(°F)
Olefins				
Ethylene-ethene	0.974	50.5	259.2	498
Propylene-propane	1.451	45.4	92.0	197
Butylene (iso) 2-methylpropane	1.934	39.5	145.3	293
Butylene (a) butene 1	1.934	39.7	147.0	296
Butylene (b) butene 2	2.004	40.8	155.3	311
Amylene (N) pentene 1	2.420	39.9	201.4	394
Diolefins				
Butadiene 1.3	1.869	42.7	152.6	306
Butadiene 1.2	1.869	—	—	—
Acetylene				
Acetylene-ethyne	0.911	61.6	36.4	97
Aromatics				
Benzene	2.692	48.6	289.8	553
Toluene-methylbenzene	3.176	40.1	321.4	610
Miscellaneous gases				
Air	1.000	37.2	−140.0	−221
Ammonia	0.596	111.5	132.6	270
Carbon monoxide	0.967	35.0	−138.6	−218
Carbon dioxide	1.528	72.9	31.4	88
Chlorine	2.449	76.0	144.2	291
Hydrogen	0.0696	12.8	−239.7	−400
Hydrogen sulfide	1.190	88.8	100.9	213
Nitrogen	0.972	33.5	−146.9	−233
Oxygen	1.105	49.7	−118.6	−182
Sulfur dioxide	2.44	77.8	157.6	315

[a]Refers to isooctane, used as a standard in fuel testing. Organic chemists apply the same name to 2-methylheptane.

Source: Flow Meter Engineering Handbook, 3rd Edition, Philadelphia, PA (1961).

Solid and liquid fuel constant volume bomb calorimetry is not used with gaseous fuels. Instead, heating values of gaseous fuels are experimentally determined using a constant pressure flow calorimeter.

The molar heat of combustion of methane, a major gaseous fuel constituent, is

$$HHV_{CH_4} = (212{,}800 \text{ cal/g mole})(4.187) = 890{,}994 \text{ kJ/kg mole} \quad (2.4a)$$

or

$$= (212{,}800 \text{ cal/g mole})(1.8001) = 383{,}040 \text{ Btu/lb mole} \quad (2.4b)$$

The molar density of methane at STP can be obtained from equation (2.2) and is equal to

$$\bar{\rho}_{CH_4} = \frac{(101{,}000\,N/m^2)}{(8314\,kNm/kgmoleK)/298K)} = 0.0408 \text{ kg mole/m}^3 \qquad (2.5a)$$

or

$$= \frac{(14{,}7lbf/in^2)(144in^2/ft^2)}{(1545\,ftlbf/lbmoleR)(537°R)} = 0.00255 \text{ lb mole/ft}^3 \qquad (2.5b)$$

By combining these equations, the volumetric heating value for methane is given as

$$\overline{HHV}_{CH_4} = (890{,}994 \text{ kJ/kg mole})(0.0408 \text{ kg mole/m}^3) = 36{,}350 \text{ kJ/m}^3 \qquad (2.6a)$$

$$= (383{,}040 \text{ Btu/lb mole})(0.00255 \text{ lb mole/ft}^3) = 977 \text{ Btu/ft}^3 \qquad (2.6b)$$

The heating value of gaseous fuel is most often specified on a per-unit volume basis, whereas solid and liquid fuels are usually expressed in terms of a unit mass of fuel. It is essential that energy for different fuels be compared on a consistent basis, i.e., per unit mole, unit volume, or unit mass. To illustrate, consider the molar heating values of methane and hydrogen:

$$\overline{HHV}_{CH_4} = 890{,}994 \text{ kJ/kg mole} \qquad (2.7a)$$

(383,040 Btu/lb mole)

and

$$\overline{HHV}_{H_2} = 286{,}043 \text{ kJ/kg mole} \qquad (2.7b)$$

(122,997 Btu/lb mole)

Equations (2.7a) and (2.7b) clearly show that, on a molar basis, methane has a greater heating value than hydrogen.

The heating value for these two fuels on a volumetric basis is equal to

$$HHV = \overline{HHV}\ \overline{\rho} \tag{2.8}$$

and

$$HHV_{CH_4} = (890{,}994)(0{,}0408) = 36{,}350 \text{ kJ/m}^3 \text{ (997 Btu/ft}^3\text{)} \tag{2.8a}$$

$$HHV_{H_2} = (286{,}043)(0{,}0408) = 11{,}670 \text{ kJ/m}^3 \text{ (314 Btu/ft}^3\text{)} \tag{2.8b}$$

Equations (2.8a) and (2.8b) show that, on a unit volume basis, methane also has a greater heating value than hydrogen.

Finally, the heating value for these two fuels on a mass basis is equal to

$$HHV = \overline{HHV} / MW \tag{2.9}$$

with

$$HHV_{CH_4} = 890{,}994/16 = 55{,}687 \text{ kJ/kg (23,940 Btu/lbm)} \tag{2.9a}$$

and

$$HHV_{H_2} = 286{,}043/2 = 143{,}022 \text{ kJ/kg (61,489 Btu/lbm)} \tag{2.9b}$$

Equations (2.9a) and (2.9b) indicate that, on a unit mass basis, however, hydrogen has a greater heating value than methane.

Propulsion heat engine utilization usually involves vehicle weight and/or volume design restrictions. In these instances, the fuel engine energy density requirements of such machinery may dictate the use of fuels having high heats of combustion on both a unit mass and volume basis. This suggests that gaseous fuels may not be suited to mobility power requirements but, instead, are more compatible with heating and stationary power needs. In addition, when the combustion characteristics of gaseous

fuels are matched with a particular gas burner, the fuel-engine energy interface requirements cannot be based on selecting fuels having an equal heating value or specific gravity alone. In fact, in order pass a constant energy rate through a given burner orifice, gaseous fuels with equal operating gas pressure levels and pressure drop across the orifice must have an equal Wobble number, W_0, where

W_0 = (higher heating value of gaseous fuel) / ($\sqrt{SG}$) (2.10)

Gaseous fuel had a greater role as a stationary power fuel because of environmental benefits associated with their clean burning until the energy crisis placed an economic premium on fuel alternatives. The concentrations of CO, CO2 and O2 in the exhaust from natural gas and even oil-fired boilers and furnaces can be measured by chemical absorption devices such as the Orsat analyzer. Exhaust, or flue, gases are monitored in many boiler applications, and major exhaust gas composition measurements via an Orsat analysis can be used to operate an efficient burner stoichiometry. A discussion of more complex and sensitive methods of analysis, such as gas chromatography, ultraviolet infrared emissions spectroscopy, ultraviolet absorption spectroscopy, and mass spectrometry, which are use to determine the presence of minute amounts of unburned hydrocarbons and nitric oxides.[2-4]

2.3. Natural Gas

The world's most readily available and abundant gaseous fuel resources are found in natural gas reserves. Gaseous fuels have been used for centuries in China and for over 100 years in both the United States and Europe. In the United States, when natural gas was originally discovered at oil wells, it was burned, or flared off, as a useless by-product of oil production. Today, natural gas is a major industry that transports fuel throughout the United States by a complex interstate pipeline network. Natural gas formed by anaerobic, or bacterial-assisted, decomposition of organic matter under heat and pressure and, therefore, like coal and crude oil, is a variable composition hydrocarbon fuel. Table 2.2 lists physical properties of natural gas.

Table 2.2. Physical properties of natural gas

Physical State	Gas (under normal conditions)
Density (kg/m^3)	0.58 – 0.79
Color and Smell	Colorless and odourless
Flame Temperature (°C) and Combustion Speed (m^3 /s)	2780 – 0.35

Natural gas consists chiefly of methane, ranging anywhere from 75% to 99% by volume, with varying concentrations of low molecular weight hydrocarbons, CO, CO_2, He, N_2 and/or H_2O. Conventional gas well drilling has proved successful in or near oil fields. New and additional unconventional drilling methods are finding reserves in deep wells and coal beds, as well as in shale and tar sands. Natural gas is practically colorless and odorless and, for safety reasons, is ‘’soured’’ with the familiar rotten egg odor by adding hydrogen sulfide, H_2S. The American Gas Association classifies natural gas as sweet and sour gas and, additionally, as being associated or non associated gas. Associated, or wet, gas is either dissolved in crude oil reserves or confined in pressurized gas caps located on the top of oil ponds. Wet gas has appreciable concentrations of ethane, butane, propane, propylene, and butylenes. Non associated, or dry, gas van be found in gas pockets trapped under high pressure that have migrated from oil ponds or are the results of an early coalization gasification stage. Natural gas, like coal and oil, has regional characteristics. For example, western U.S. natural gas fields generally contain substantial amounts of CO_2, Midwestern reserves have higher N_2 concentrations and some He, and eastern gas is high in paraffin. European gas reserves are basically high in CO_2, H_2, and olefin hydrocarbons.

Liquid petroleum gas, or LPG, consists of condensable hydrocarbon vapors recovered by expansion of wet gas reserves. By compressing the condensable fractions, liquefied liquid vapors, such as commercial propane and butane, can be stored and transported at ambient temperatures as a liquid. Liquefied natural gas, LNG, is the condensed state of dry natural gas but requires cryogenic refrigeration for storage and handling at -102°C (-260°F). At present, efficient transportation of

large Middle Eastern natural gas to the United States, Europe and Asia by sea requires specially designed LNG tankers.[2-4,6-7]

2.4. Liquid And Gaseous Fuel Burners

Solid fuels have been replaced today in most heat and/or power applications by liquid and gaseous hydrocarbon fuels. This is due, in part, to the thermo chemical properties and portable nature of fuels, which allow such materials to be easily stored, transported, handled, and prepared for combustion. Note that liquid and gaseous fuel delivery components will be simpler than those systems for use with solid fuels. In addition, the required reaction volume for burning fuel oil or gas is considerably less than that needed for most solid fuel reactions. Commercial use of liquid and/or gaseous fuels for heat transfer applications, such as space or industrial process heating, and/or steam generation, requires burners that will sustain atmospheric combustion within a particular furnace or even.

Specific burner-fuel interactions are strongly influenced by properties of the particular fuel being fired. For example, the basic elements needed to properly and efficiently burn fuel oils using a burner are:

- Proper and safe storage of the fuel
- Settling equipment as well as fuel filters and strainers to ensure constant fuel quality
- Use of fuel heaters when necessary, such as when burning heavy fuel oils
- Suitable fuel delivery pumps to ensure consistent and sufficient fuel flow
- Suitable furnace volume for complete combustion
- Burner elements that supply fuel to the furnace by
    - Injecting atomized fuel oil droplets
    - Vaporizing fuel and preheating fuel vapor
    - Mixing with sufficient air for combustion
    - Igniting the fuel-air mixture

An essential requirement of any oil-burning system is to ensure that fuel is supplied at a proper temperature, pressure, and viscosity to enable the burner to mix suitably atomized fuel into air to combustion. Oil burner designs basically consist of two parts; a burner barrel, or atomizer, which allows a stream of small droplets of fuel to be supplied to the combustion chamber, and a register, which supplies as well as

regulates combustion air to the furnace. Some burners use mechanical techniques, such as a high pressure fuel supply, to produce atomized fuel oil. Other designs use fluid techniques, such as high pressure fuel and air or fuel and steam injection to generate atomized fuel droplets. Several types of oil burners have found use and include swirl atomizers, rotary cup burners, and high pressure jet atomizers.

Gaseous fuels do not require charge preparation since they already exist naturally in a reactive state. The main function of the gas burner is therefore to introduce the fuel at the proper AF ratio.

Gas burners are either low and high pressure configurations. Low pressure units are most frequently used with natural gas systems that are generally found in domestic applications, such as cooking and heating. These burners, often located near the floor level of the unit, use a multi-jet arrangement to discharge fuel gas vertically into the furnace. Combustion air allows around the burner orifices and fuel-air ignition and combustion then occur above the burner. High pressure gas burner designs were incorporated in certain steam generation plants by the 1920s to 1930s in regions where natural gas was available.

An important operational parameter for a particular burner is its turndown ratio, i.e., the ratio of maximum fuel input rate to minimum fuel input. The upper range of this parameter is limited by incomplete combustion, blow off, or inability to supply sufficient primary air. The lower limit is governed by the extinction of the flame or flashback tendency of the reaction zone. Turndown ranges in excess of 5 to 1 are usually difficult to sustain.[3]

3. COMBUSTION

3.1. Combustion Of Hydrocarbons

Combustion is a physical and chemical phenomenon during which the chemical energy is released thermal energy as a result of the reaction between fuel and oxidizer. Fuel may contain many kinds of chemical species that consist of many kinds of chemical elements. More than 90% of fuel used as energy source is based on carbon and hydrogen and more than 90% of oxidizer used in combustion is the oxygen of the ambient air. However, there are some reactions between other kind chemical species or elements that we may also call combustion.

The common property of the reactions that we may consider is a net heat release. The heat release due to the positive difference of the chemical bond energy between the initial species (fuel + oxidizer or reactants) and the final species (products).

Combustion begins from the initial state (of reactants) and proceeds in time to the final state (of products) via various intermediate reactions and species. However, for the first step, it is more practical to assume the reactions to occur with infinite rate and consider only the reactants and the final products. This approach gives us the opportunity to analyse the combustion system in a much easier way, using only the classical conservation laws and the algebraic equations between temperature and species concentrations. However, it is of course necessary in many cases to analyse the real physical combustion process using the governing differential equations of time, concentrations and temperature.

Combustion equilibrium of general hydrocarbon fuel (C_nH_m) and oxygen (O_2) mixture is:

$$C_nH_m + (n + \frac{m}{4})\, O_2 \rightarrow n\, CO_2 + \frac{m}{2}\, H_2O$$

This means that (n + $\frac{m}{4}$) moles of oxygen are required to burn one mole of fuel (C_nH_m) completely.[8]

3.2. Combustion Of Methane

Combustion is a chemical phenomenon. Carbon and hydrogen that are contained by fuel produce thermal energy reacting air. It is seems with this expression that carbon and hydrogen are the burning elements of liquid fuels.

The oxygen is provided from the ambient air. Air is a mixture of the gaseous that are oxygen, nitrogen, and carbon dioxide, less amount of water vapor and waste gaseous. It is accepted that air is formed by 21% oxygen and 79% nitrogen volumetrically due to the amount of the carbon dioxide and waste gaseous are little.

During combustion, fuel particles are split into hydrogen and carbon atoms, and every elements combine with oxygen of the air. Hydrogen and oxygen generate water vapor; carbon and oxygen produce carbon dioxide. Carbon monoxide would be occurred if there was insufficient oxygen.

When carbon burns, CO or CO_2 be formed depends on combustion conditions. CO is formed when the fuel react with limited oxygen, CO_2 is formed when combustion occur with abundant oxygen.

$$2C + O_2 \rightarrow 2CO$$

formed CO could be burned with oxygen;

$$2CO + O_2 \rightarrow 2CO_2$$

Carbon and hydrogen components are named as hydrocarbons and they are important fuels. The simplest of them is CH_4, methane. Methane is the most important component of natural gas and it is very important fuel. When hydrocarbon burns, CO, CO_2 and water be formed. C, CO_2 and/or CO is formed depends on the amount of oxygen.

$CH_4 + O_2 \rightarrow C + 2H_2O$

The reaction above is occurred when the mixture is excessive rich.

state of lean mixture;

$2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O$

state of rich mixture;

$CH_4 + O_2 \rightarrow CO_2 + 2H_2$

Methane is colorless and odorless, and is being in abundant amount in the nature. It is the main element of natural gas. Methane is low concentrated than air under normal conditions. That is melted at -183°C, boiled at -164°C. Its solubility is not good in the water. Methane is burnable; if there was 5-15% methane in the air, it would be explosive. Methane has no poison effect, but suffocating. Dimetil sulphur (CH_3-S-CH_3) is added in order to make clear its odor.

Methane is used as fuel commonly. Combustion of methane is highly exothermic.

$CH_4 + 2O_2 \rightarrow CO_2 + H_2O$ $\Delta H = -891kJ$

The thermal energy that is obtained from methane combustion is used in heating applications of homes and buildings. It is possible to produce electricity via this exothermic reaction. Natural gas has been covering 1/5 of world's energy consumption and 1/3 of energy consumption in America for ten years. [4,9,10]

3.2.1.Complex mechanism

Because of its unique tetrahedral molecular structure with large C-H bond energies, methane exhibits some unique combustion characteristics. For example, it has a high

ignition temperature, low flame speed, and is essentially unreactive in photochemical smog chemistry.

Methane chemical kinetics are perhaps the most widely researched and, hence, most well understood. In a revive of combustion kinetics indicated that he methane combustion mechanism evolved in the period 1970-1982 from less than 15 elementary steps with 12 species to 75 elementary steps, plus the 75 reverse reactions, with 25 species. Recently, several research groups have collaborated in the creation of an optimized methane kinetic mechanism. This mechanism, designated GRI Mech, is based on the optimization techniques of Frenklach. In Table 3.1 325 elementary reactions is shown. Many of these steps we know as part of the H_2 and CO oxidation mechanisms. [10]

Table 3.1. Complex methane combustion mechanism [11]

Number	**Reaction**	**Rate Coefficient** $A\,T^n\,exp^{(-E/RT)}$		
		A **(mol,cm^3,s)**	**n** **(T in K)**	**E** **(cal/mol)**
1	O + O + M -> O_2 + M	1.20E+17	-1.0	
2	O + H + M -> OH + M	5.00E+17	-1.0	
3	O + H_2 -> H + OH	3.87E+04	2.7	6260
4	O + HO_2 -> OH + O_2	2.00E+13		
5	O + H_2O_2 -> OH + HO_2	9.63E+06	2.0	4000
6	O + CH -> H + CO	5.70E+13		
7	O + CH_2 -> H + HCO	8.00E+13		

8	$O + CH_2(S) \rightarrow H_2 + CO$	1.50E+13		
9	$O + CH_2(S) \rightarrow H + HCO$	1.50E+13		
10	$O + CH_3 \rightarrow H + CH_2O$	5.06E+13		
11	$O + CH_4 \rightarrow OH + CH_3$	1.02E+09	1.5	8600
12	$O + CO + M \rightarrow CO_2 + M$	1.80E+10		2385
13	$O + HCO \rightarrow OH + CO$	3.00E+13		
14	$O + HCO \rightarrow H + CO_2$	3.00E+13		
15	$O + CH_2O \rightarrow OH + HCO$	3.90E+13		3540
16	$O + CH_2OH \rightarrow OH + CH_2O$	1.00E+13		
17	O + CH3O -> OH + CH2O	1.00E+13		
18	O + CH3OH > OH + CH2OH	3.88E+05	2.5	3100
19	O + CH3OH -> OH + CH3O	1.30E+05	2.5	5000
20	O + C2H -> CH + CO	5.00E+13		
21	O + C2H2 -> H + HCCO	1.35E+07	2.0	1900
22	O + C2H2 -> OH + C2H	4.60E+19	-1.4	28950
23	O + C2H2 -> CO + CH2	6.94E+06	2.0	1900

24	O + C2H3 -> H + CH2CO	3.00E+13		
25	O + C2H4 -> CH3 + HCO	1.25E+07	1.8	220
26	O + C2H5 -> CH3 + CH2O	2.24E+13		
27	O + C2H6 -> OH + C2H5	8.98E+07	1.9	5690
28	O + HCCO -> H + CO + CO	1.00E+14		
29	O + CH2CO -> OH + HCCO	1.00E+13		8000
30	O + CH2CO -> CH2 + CO2	1.75E+12		1350
31	O2 + CO -> O + CO2	2.50E+12		47800
32	O2 + CH2O -> HO2 + HCO	1.00E+14		40000
33	H + O2 + M -> HO2 + M	2.80E+18	-0.9	
34	H + O2 + O2 -> HO2 + O2	2.08E+19	-1.2	
35	H + O2 + H2O > HO2 + H2O	1.13E+19	-0.8	
36	H + O2 + N2 -> HO2 + N2	2.60E+19	-1.2	
37	H + O2 + AR -> HO2 + AR	7.00E+17	-0.8	
38	H + O2 -> O + OH	2.65E+16	-0.7	17041
39	H + H + M -> H2 + M	1.00E+18	-1.0	

40	H + H + H2 -> H2 + H2	9.00E+16	-0.6	
41	H + H + H2O -> H2 + H2O	6.00E+19	-1.2	
42	H + H + CO2 -> H2 + CO2	5.50E+20	-2.0	
43	H + OH + M -> H2O + M	2.20E+22	-2.0	
44	H + HO2 -> O + H2O	3.97E+12		671
45	H + HO2 -> O2 + H2	4.48E+13		1068
46	H + HO2 -> OH + OH	8.40E+13		635
47	H + H2O2 -> HO2 + H2	1.21E+07	2.0	5200
48	H + H2O2 -> OH + H2O	1.00E+13		3600
49	H + CH -> C + H2	1.65E+14		
50	H + CH2 (+M) -> CH3 (+M)	pressure dependent		
51	H + CH2(S) -> CH + H2	3.00E+13		
52	H + CH3 (+M) -> CH4 (+M)	pressure dependent		
53	H + CH4 -> CH3 + H2	6.60E+08	1.6	10840
54	H + HCO (+M) > CH2O (+M)	pressure dependent		
55	H + HCO -> H2 + CO	7.34E+13		

56	H + CH2O (+M) -> CH2OH (+M)	pressure dependent		
57	H + CH2O (+M) > CH3O (+M)	pressure dependent		
58	H + CH2O -> HCO + H2	5.74E+07	1.9	2742
59	H + CH2OH (+M) > CH3OH (+M)	pressure dependent		
60	H + CH2OH -> H2 + CH2O	2.00E+13		
61	H + CH2OH -> OH + CH3	1.65E+11	0.7	-284
62	H + CH2OH -> CH2(S) + H2O	3.28E+13	-0.1	610
63	H + CH3O (+M) -> CH3OH (+M)	pressure dependent		
64	H + CH3O -> H + CH2OH	4.15E+07	1.6	1924
65	H + CH3O -> H2 + CH2O	2.00E+13		
66	H + CH3O -> OH + CH3	1.50E+12	0.5	-110
67	H + CH3O -> CH2(S) + H2O	2.62E+14	-0.2	1070
68	H + CH3OH -> CH2OH + H2	1.70E+07	2.1	4870
69	H + CH3OH -> CH3O + H2	4.20E+06	2.1	4870
70	H + C2H (+M) -> C2H2 (+M)	pressure dependent		
71	H + C2H2 (+M) -> C2H3 (+M)	pressure dependent		

72	H + C2H3 (+M) -> C2H4 (+M)	pressure dependent		
73	H + C2H3 -> H2 + C2H2	3.00E+13		
74	H + C2H4 (+M) -> C2H5 (+M)	pressure dependent		
75	H + C2H4 -> C2H3 + H2	1.32E+06	2.5	12240
76	H + C2H5 (+M) -> C2H6 (+M)	pressure dependent		
77	H + C2H5 -> H2 + C2H4	2.00E+12		
78	H + C2H6 -> C2H5 + H2	1.15E+08	1.9	7530
79	H + HCCO > CH2(S) + CO	1.00E+14		
80	H + CH2CO > HCCO + H2	5.00E+13		8000
81	H + CH2CO -> CH3 + CO	1.13E+13		3428
82	H + HCCOH -> H + CH2CO	1.00E+13		
83	H2 + CO (+M) -> CH2O (+M)	pressure dependent		
84	OH + H2 -> H + H2O	2.16E+08	1.5	3430
85	OH + OH (+M) -> H2O2 (+M)	pressure dependent		
86	OH + OH -> O + H2O	3.57E+04	2.4	-2110
87	OH + HO2 -> O2 + H2O	1.45E+13		-500

88	OH + H2O2 -> HO2 + H2O	2.00E+12		427
89	OH + H2O2 -> HO2 + H2O	1.70E+18		29410
90	OH + C -> H + CO	5.00E+13		
91	OH + CH -> H + HCO	3.00E+13		
92	OH + CH2 -> H + CH2O	2.00E+13		
93	OH + CH2 -> CH + H2O	1.13E+07	2.0	3000
94	OH + CH2(S) -> H + CH2O	3.00E+13		
95	OH + CH3 (+M) -> CH3OH (+M)	pressure dependent		
96	OH + CH3 -> CH2 + H2O	5.60E+07	1.6	5420
97	OH + CH3 -> CH2(S) + H2O	6.44E+17	-1.3	1417
98	OH + CH4 -> CH3 + H2O	1.00E+08	1.6	3120
99	OH + CO -> H + CO2	4.76E+07	1.2	70
100	OH + HCO -> H2O + CO	5.00E+13		
101	OH + CH2O -> HCO + H2O	3.43E+09	1.2	-447
102	OH + CH2OH -> H2O + CH2O	5.00E+12		
103	OH + CH3O -> H2O + CH2O	5.00E+12		

104	OH + CH3OH -> CH2OH + H2O	1.44E+06	2.0	-840
105	OH + CH3OH -> CH3O + H2O	6.30E+06	2.0	1500
106	OH + C2H -> H + HCCO	2.00E+13		
107	OH + C2H2 -> H + CH2CO	2.18E-04	4.5	-1000
108	OH + C2H2 -> H + HCCOH	5.04E+05	2.3	13500
109	OH + C2H2 -> C2H + H2O	3.37E+07	2.0	14000
110	OH + C2H2 -> CH3 + CO	4.83E-04	4.0	-2000
111	OH + C2H3 -> H2O + C2H2	5.00E+12		
112	OH + C2H4 -> C2H3 + H2O	3.60E+06	2.0	2500
113	OH + C2H6 -> C2H5 + H2O	3.54E+06	2.1	870
114	OH + CH2CO -> HCCO + H2O	7.50E+12		2000
115	HO2 + HO2 -> O2 + H2O2	1.30E+11		-1630
116	HO2 + HO2 -> O2 + H2O2	4.20E+14		12000
117	HO2 + CH2 -> OH + CH2O	2.00E+13		
118	HO2 + CH3 -> O2 + CH4	1.00E+12		
119	HO2 + CH3 -> OH + CH3O	3.78E+13		

120	HO2 + CO -> OH + CO2	1.50E+14		23600
121	HO2 + CH2O -> HCO + H2O2	5.60E+06	2.0	12000
122	C + O2 -> O + CO	5.80E+13		576
123	C + CH2 -> H + C2H	5.00E+13		
124	C + CH3 -> H + C2H2	5.00E+13		
125	CH + O2 -> O + HCO	6.71E+13		
126	CH + H2 -> H + CH2	1.08E+14		3110
127	CH + H2O -> H + CH2O	5.71E+12		-755
128	CH + CH2 -> H + C2H2	4.00E+13		
129	CH + CH3 -> H + C2H3	3.00E+13		
130	CH + CH4 -> H + C2H4	6.00E+13		
131	CH + CO (+M) -> HCCO (+M)	pressure dependent		
132	CH + CO2 -> HCO + CO	1.90E+14		15792
133	CH + CH2O -> H + CH2CO	9.46E+13		-515
134	CH + HCCO -> CO + C2H2	5.00E+13		
135	CH2 + O2 -> OH + H + CO	5.00E+12		1500

136	CH2 + H2 -> H + CH3	5.00E+05	2.0	7230
137	CH2 + CH2 -> H2 + C2H2	1.60E+15		11944
138	CH2 + CH3 -> H + C2H4	4.00E+13		
139	CH2 + CH4 -> CH3 + CH3	2.46E+06	2.0	8270
140	CH2 + CO (+M) -> CH2CO (+M)	pressure dependent		
141	CH2 + HCCO -> C2H3 + CO	3.00E+13		
142	CH2(S) + N2 -> CH2 + N2	1.50E+13		600
143	CH2(S) + AR -> CH2 + AR	9.00E+12		600
144	CH2(S) + O2 -> H + OH + CO	2.80E+13		
145	CH2(S) + O2 -> CO + H2O	1.20E+13		
146	CH2(S) + H2 -> CH3 + H	7.00E+13		
147	CH2(S) + H2O (+M) > CH3OH (+M)	pressure dependent		
148	CH2(S) + H2O -> CH2 + H2O	3.00E+13		
149	CH2(S) + CH3 -> H + C2H4	1.20E+13		-570
150	CH2(S) + CH4 -> CH3 + CH3	1.60E+13		-570
151	CH2(S) + CO -> CH2 + CO	9.00E+12		

152	CH2(S) + CO2 -> CH2 + CO2	7.00E+12		
153	CH2(S) + CO2 -> CO + CH2O	1.40E+13		
154	CH2(S) + C2H6 -> CH3 + C2H5	4.00E+13		-550
155	CH3 + O2 -> O + CH3O	3.56E+13		30480
156	CH3 + O2 -> OH + CH2O	2.31E+12		20315
157	CH3 + H2O2 -> HO2 + CH4	2.45E+04	2.5	5180
158	CH3 + CH3 (+M) -> C2H6 (+M)	pressure dependent		
159	CH3 + CH3 -> H + C2H5	6.84E+12	0.1	10600
160	CH3 + HCO -> CH4 + CO	2.65E+13		
161	CH3 + CH2O -> HCO + CH4	3.32E+03	2.8	5860
162	CH3 + CH3OH -> CH2OH + CH4	3.00E+07	1.5	9940
163	CH3 + CH3OH -> CH3O + CH4	1.00E+07	1.5	9940
164	CH3 + C2H4 -> C2H3 + CH4	2.27E+05	2.0	9200
165	CH3 + C2H6 -> C2H5 + CH4	6.14E+06	1.7	10450
166	HCO + H2O -> H + CO + H2O	1.50E+18	-1.0	17000
167	HCO + M -> H + CO + M	1.87E+17	-1.0	17000

168	HCO + O2 -> HO2 + CO	1.35E+13		400
169	CH2OH + O2 -> HO2 + CH2O	1.80E+13		900
170	CH3O + O2 -> HO2 + CH2O	4.28E-13	7.6	-3530
171	C2H + O2 -> HCO + CO	1.00E+13		-755
172	C2H + H2 -> H + C2H2	5.68E+10	0.9	1993
173	C2H3 + O2 -> HCO + CH2O	4.58E+16	-1.4	1015
174	C2H4 (+M) -> H2 + C2H2 (+M)	pressure dependent		
175	C2H5 + O2 -> HO2 + C2H4	8.40E+11		3875
176	HCCO + O2 -> OH + CO + CO	3.20E+12		854
177	HCCO + HCCO > CO + CO + C2H2	1.00E+13		
178	N + NO -> N2 + O	2.70E+13		355
179	N + O2 -> NO + O	9.00E+09	1.0	6500
180	N + OH -> NO + H	3.36E+13		385
181	N2O + O -> N2 + O2	1.40E+12		10810
182	N2O + O -> NO + NO	2.90E+13		23150
183	N2O + H -> N2 + OH	3.87E+14		18880

184	N2O + OH -> N2 + HO2	2.00E+12		21060
185	N2O (+M) -> N2 + O (+M)	pressure dependent		
186	HO2 + NO -> NO2 + OH	2.11E+12		-480
187	NO + O + M -> NO2 + M	1.06E+20	-1.4	
188	NO2 + O -> NO + O2	3.90E+12		-240
189	NO2 + H -> NO + OH	1.32E+14		360
190	NH + O -> NO + H	4.00E+13		
191	NH + H -> N + H2	3.20E+13		330
192	NH + OH -> HNO + H	2.00E+13		
193	NH + OH -> N + H2O	2.00E+09	1.2	
194	NH + O2 -> HNO + O	4.61E+05	2.0	6500
195	NH + O2 -> NO + OH	1.28E+06	1.5	100
196	NH + N -> N2 + H	1.50E+13		
197	NH + H2O -> HNO + H2	2.00E+13		13850
198	NH + NO -> N2 + OH	2.16E+13	-0.2	
199	NH + NO -> N2O + H	3.65E+14	-0.5	

200	NH2 + O -> OH + NH	3.00E+12		
201	NH2 + O -> H + HNO	3.90E+13		
202	NH2 + H -> NH + H2	4.00E+13		3650
203	NH2 + OH -> NH + H2O	9.00E+07	1.5	-460
204	NNH -> N2 + H	3.30E+08		
205	NNH + M -> N2 + H + M	1.30E+14	-0.1	4980
206	NNH + O2 -> HO2 + N2	5.00E+12		
207	NNH + O -> OH + N2	2.50E+13		
208	NNH + O -> NH + NO	7.00E+13		
209	NNH + H -> H2 + N2	5.00E+13		
210	NNH + OH -> H2O + N2	2.00E+13		
211	NNH + CH3 -> CH4 + N2	2.50E+13		
212	H + NO + M -> HNO + M	4.48E+19	-1.3	740
213	HNO + O -> NO + OH	2.50E+13		
214	HNO + H -> H2 + NO	9.00E+11	0.7	660
215	HNO + OH -> NO + H2O	1.30E+07	1.9	-950

216	HNO + O2 -> HO2 + NO	1.00E+13		13000
217	CN + O -> CO + N	7.70E+13		
218	CN + OH -> NCO + H	4.00E+13		
219	CN + H2O -> HCN + OH	8.00E+12		7460
220	CN + O2 -> NCO + O	6.14E+12		-440
221	CN + H2 -> HCN + H	2.95E+05	2.5	2240
222	NCO + O -> NO + CO	2.35E+13		
223	NCO + H -> NH + CO	5.40E+13		
224	NCO + OH -> NO + H + CO	2.50E+12		
225	NCO + N -> N2 + CO	2.00E+13		
226	NCO + O2 -> NO + CO2	2.00E+12		20000
227	NCO + M -> N + CO + M	3.10E+14		54050
228	NCO + NO -> N2O + CO	1.90E+17	-1.5	740
229	NCO + NO -> N2 + CO2	3.80E+18	-2.0	800
230	HCN + M -> H + CN + M	1.04E+29	-3.3	126600
231	HCN + O -> NCO + H	2.03E+04	2.6	4980

232	HCN + O -> NH + CO	5.07E+03	2.6	4980
233	HCN + O -> CN + OH	3.91E+09	1.6	26600
234	HCN + OH -> HOCN + H	1.10E+06	2.0	13370
235	HCN + OH -> HNCO + H	4.40E+03	2.3	6400
236	HCN + OH -> NH2 + CO	1.60E+02	2.6	9000
237	H + HCN (+M) -> H2CN (+M)	pressure dependent		
238	H2CN + N -> N2 + CH2	6.00E+13		400
239	C + N2 -> CN + N	6.30E+13		46020
240	CH + N2 -> HCN + N	3.12E+09	0.9	20130
241	CH + N2 (+M) -> HCNN (+M)	pressure dependent		
242	CH2 + N2 -> HCN + NH	1.00E+13		74000
243	CH2(S) + N2 -> NH + HCN	1.00E+11		65000
244	C + NO -> CN + O	1.90E+13		
245	C + NO -> CO + N	2.90E+13		
246	CH + NO -> HCN + O	4.10E+13		
247	CH + NO -> H + NCO	1.62E+13		

248	CH + NO -> N + HCO	2.46E+13		
249	CH2 + NO -> H + HNCO	3.10E+17	-1.4	1270
250	CH2 + NO -> OH + HCN	2.90E+14	-0.7	760
251	CH2 + NO -> H + HCNO	3.80E+13	-0.4	580
252	CH2(S) + NO -> H + HNCO	3.10E+17	-1.4	1270
253	CH2(S) + NO -> OH + HCN	2.90E+14	-0.7	760
254	CH2(S) + NO -> H + HCNO	3.80E+13	-0.4	580
255	CH3 + NO -> HCN + H2O	9.60E+13		28800
256	CH3 + NO -> H2CN + OH	1.00E+12		21750
257	HCNN + O -> CO + H + N2	2.20E+13		
258	HCNN + O -> HCN + NO	2.00E+12		
259	HCNN + O2 -> O + HCO + N2	1.20E+13		
260	HCNN + OH -> H + HCO + N2	1.20E+13		
261	HCNN + H -> CH2 + N2	1.00E+14		
262	HNCO + O -> NH + CO2	9.80E+07	1.4	8500
263	HNCO + O -> HNO + CO	1.50E+08	1.6	44000

264	HNCO + O -> NCO + OH	2.20E+06	2.1	11400
265	HNCO + H -> NH2 + CO	2.25E+07	1.7	3800
266	HNCO + H -> H2 + NCO	1.05E+05	2.5	13300
267	HNCO + OH -> NCO + H2O	3.30E+07	1.5	3600
268	HNCO + OH -> NH2 + CO2	3.30E+06	1.5	3600
269	HNCO + M -> NH + CO + M	1.18E+16		84720
270	HCNO + H -> H + HNCO	2.10E+15	-0.7	2850
271	HCNO + H -> OH + HCN	2.70E+11	0.2	2120
272	HCNO + H -> NH2 + CO	1.70E+14	-0.8	2890
273	HOCN + H -> H + HNCO	2.00E+07	2.0	2000
274	HCCO + NO -> HCNO + CO	9.00E+12		
275	CH3 + N -> H2CN + H	6.10E+14	-0.3	290
276	CH3 + N -> HCN + H2	3.70E+12	0.1	-90
277	NH3 + H -> NH2 + H2	5.40E+05	2.4	9915
278	NH3 + OH -> NH2 + H2O	5.00E+07	1.6	955
279	NH3 + O -> NH2 + OH	9.40E+06	1.9	6460

280	NH + CO2 -> HNO + CO	1.00E+13		14350
281	CN + NO2 -> NCO + NO	6.16E+15	-0.8	345
282	NCO + NO2 -> N2O + CO2	3.25E+12		-705
283	N + CO2 -> NO + CO	3.00E+12		11300
284	O + CH3 -> H + H2 + CO	3.37E+13		
285	O + C2H4 -> H + CH2CHO	6.70E+06	1.8	220
286	O + C2H5 -> H + CH3CHO	1.10E+14		
287	OH + HO2 -> O2 + H2O	5.00E+15		17330
288	OH + CH3 -> H2 + CH2O	8.00E+09	0.5	-1755
289	CH + H2 (+M) -> CH3 (+M)	pressure dependent		
290	CH2 + O2 -> H + H + CO2	5.80E+12		1500
291	CH2 + O2 -> O + CH2O	2.40E+12		1500
292	CH2 + CH2 -> H + H + C2H2	2.00E+14		10989
293	CH2(S) + H2O -> H2 + CH2O	6.82E+10	0.2	-935
294	C2H3 + O2 -> O + CH2CHO	3.03E+11	0.3	11
295	C2H3 + O2 -> HO2 + C2H2	1.34E+06	1.6	-384

296	O + CH3CHO -> OH + CH2CHO	2.92E+12		1808
297	O + CH3CHO -> OH + CH3 + CO	2.92E+12		1808
298	O2 + CH3CHO -> HO2 + CH3 + CO	3.01E+13		39150
299	H + CH3CHO -> CH2CHO + H2	2.05E+09	1.2	2405
300	H + CH3CHO -> CH3 + H2 + CO	2.05E+09	1.2	2405
301	OH + CH3CHO -> CH3 + H2O + CO	2.34E+10	0.7	-1113
302	HO2 + CH3CHO > CH3 + H2O2 + CO	3.01E+12		11923
303	CH3 + CH3CHO -> CH3 + CH4 + CO	2.72E+06	1.8	5920
304	H + CH2CO (+M) -> CH2CHO (+M)	pressure dependent		
305	O + CH2CHO -> H + CH2 + CO2	1.50E+14		
306	O2 + CH2CHO -> OH + CO + CH2O	1.81E+10		
307	O2 + CH2CHO -> OH + HCO + HCO	2.35E+10		
308	H + CH2CHO -> CH3 + HCO	2.20E+13		
309	H + CH2CHO -> CH2CO + H2	1.10E+13		
310	OH + CH2CHO -> H2O + CH2CO	1.20E+13		
311	OH + CH2CHO -> HCO + CH2OH	3.01E+13		

312	CH3 + C2H5 (+M) -> C3H8 (+M)	pressure dependent		
313	O + C3H8 -> OH + C3H7	1.93E+05	2.7	3716
314	H + C3H8 -> C3H7 + H2	1.32E+06	2.5	6756
315	OH + C3H8 -> C3H7 + H2O	3.16E+07	1.8	934
316	C3H7 + H2O2 -> HO2 + C3H8	3.78E+02	2.7	1500
317	CH3 + C3H8 -> C3H7 + CH4	9.03E-01	3.6	7154
318	CH3 + C2H4 (+M) -> C3H7 (+M)	pressure dependent		
319	O + C3H7 -> C2H5 + CH2O	9.64E+13		
320	H + C3H7 (+M) -> C3H8 (+M)	pressure dependent		
321	H + C3H7 -> CH3 + C2H5	4.06E+06	2.2	890
322	OH + C3H7 -> C2H5 + CH2OH	2.41E+13		
323	HO2 + C3H7 -> O2 + C3H8	2.55E+10	0.3	-943
324	HO2 + C3H7 -> OH + C2H5 + CH2O	2.41E+13		
325	CH3 + C3H7 -> C2H5 + C2H5	1.93E+13	-0.3	

3.2.2. Reduced mechanism

3.2.2.1. Basic reduced mechanism

Reduced mechanism was found out from skeleton mechanism in order to modeling combustion chemistry. It would be surprising to see that reduced mechanism was taken out from methane, not hydrogen. The flame level of methane is less than hydrogen because methane chemical bonds can be exterminated easier, so that's why the mechanism found out using methane. The preheated region of methane-air mixture will be steady and constant as a result of this bond refraction. These effects make simpler analyzing methane flame at the same time. Table 3.2 shows the mechanism.

Table 3.2. Basic Reduced Mechanism

Number	Global Reaction
I	$CH_4 + 2H + H_2O \rightarrow 4H_2 + CO$
II	$H_2O + CO \rightarrow H_2 + CO_2$
III	$2H \rightarrow H_2$
IV	$O_2 + 3H_2 \rightarrow 2H_2O + 2H$
V	$H_2 + 2CO \rightarrow C_2H_2 + O_2$
VI	$N_2 + O_2 \rightarrow 2NO$
VII	$3H_2 + CO + NO \rightarrow HCN + 2H_2O + H$
VIII	$H + H_2O + CO + NO \rightarrow HNCO + O_2 + H_2$
IX	$NH_3 + H + H_2O \rightarrow NO + 3\,H_2$
X	$N_2 + H_2O \rightarrow N_2O + H_2$
XI	$NO + 2H_2 + O_2 \rightarrow NO_2 + H_2O + 2H$

3.2.2.4. Other reduced mechanisms

These mechanisms can be obtained by three ways:

a. 5 step reduced mechanism

b. 6 step reduced mechanism

c. 11 step reduced mechanism

Nitrogen reactions have not been investigated in this study. 6 step and 11 step mechanisms have not been examined, because they include nitrogen reactions. Table 3.3. indicates 5 step mechanisms.

Table 3.3. 5 Step Reduced Mechanism

Number	Global Reaction
I	$CH_4 + 2H + H_2O \rightarrow 4H_2 + CO$
II	$H_2O + CO \rightarrow H_2 + CO_2$
III	$2H \rightarrow H_2$
IV	$O_2 + 3H_2 \rightarrow 2H_2O + 2H$
V	$H_2 + 2CO \rightarrow C_2H_2 + O_2$

There is another reduced mechanism shown in Table 3.4., 4 step Seshadri-Peters mechanism that was found out by Smooke and Giovangigli in 1991, it also has not any info about NO_x chemistry.

Table 3.4. Seshadri –Peters Mechanism

Number	Global Reaction
I	$CH_4 + 2H + H_2O \rightarrow 4H_2 + CO$
II	$H_2O + CO \Leftrightarrow H_2 + CO_2$
III	$H + H + M \rightarrow H_2 + M$
IV	$O_2 + 3H_2 \Leftrightarrow 2H_2O + 2H$

In this mechanism first reaction defined as bond breaking reaction symbolizing the reactions among the root elements. Second reaction shows the oxidation of CO to produce its last product CO_2 . Third presents the connection of third degree masses and the little heat release due to this connection. Forth symbolizes that the chain getting complicated. To simplify the phenomenon, first and third reactions assumed as non-reversible.[12-14]

4. CFD AND SIMULATION

4.1. CFD

4.1.1. Definition of CFD

First, the words should be broken down:
Computational - having to do with mathematics, computation
Fluid Dynamics - the dynamics of things that flow

CFD is a computational technology that enables researchers to study the dynamics of things that flow. Using CFD, a computational model that represents a system or device that is wanted to study can be built. Then the fluid flow physics will be applied to this virtual prototype, and the software outputs a prediction of the fluid dynamics. CFD is a sophisticated analysis technique. It not only predicts fluid flow behavior, but also the transfer of heat, mass (such as in perspiration or dissolution), phase change (such as in freezing or boiling), chemical reaction (such as combustion), mechanical movement (such as an impeller turning), and stress or deformation of related solid structures (such as a mast bending in the wind).[15]

4.1.2. Benefits of CFD

Basically, the compelling reasons to use CFD are these three:

1.Insight
There are many devices and systems that are very difficult to prototype. Often, CFD analysis shows you parts of the system or phenomena happening within the system that would not otherwise be visible through any other means. CFD gives a means of visualizing and enhanced understanding of designs.

2.Foresight
Because CFD is a tool for predicting what will happen under a given set of circumstances, it can answer many ‘what if?’ questions very quickly. Some variables

can be given. It gives researcher outcomes. In a short time, it can be predicted how design will perform, and test many variations until search arrive at an optimal result. All of this is done before physical prototyping and testing. The foresight gained from CFD helps to design better and faster.

3.Efficiency
Better and faster design or analysis leads to shorter design cycles. Time and money are saved. Products get to market faster. Equipment improvements are built and installed with minimal downtime. CFD is a tool for compressing the design and development cycle.[15]

4.2. Combustion Modeling In Fluent

4.2.1. Applications

- Wide range of homogeneous and heterogeneous reacting flows

  Furnaces

  Boilers

  Process heaters

  Gas turbines
  Rocket engines

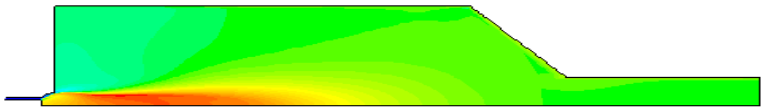
- Predictions of:

  Flow field and mixing characteristics

  Temperature field

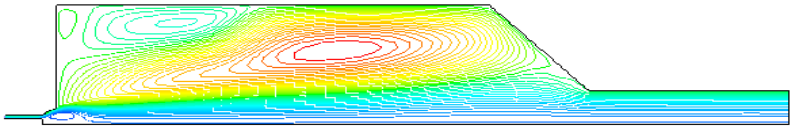
  Species concentrations
  Particulates and pollutants

Some of the applications above are shown in Figure 4.1.



Temperature in a gas furnace

CO_2 mass



Stream function

Figure 4.1. Some Fluent Applications [15]

4.2.2. Aspects in combustion modeling

a- Dispersed Phase Model

Droplet/particle dynamics

Heterogeneous reaction

Devolatilization

Evaporation

b- Combustion Models

Premixed

Partially premixed

Nonpremixed

c- Governing Transport Equations

Mass

Momentum (turbulence)

Energy

Chemical Species

d- Pollutant Models

e- Radiative Heat Transfer Models

4.2.3. Combustion models available in FLUENT

- Gas phase combustion
    - Generalized finite rate formulation (Magnussen model)
    - Conserved scalar PDF model (one and two mixture fractions)
    - Laminar flamelet model (V5)
    - Zimont model (V5)
- Discrete phase model
    - Turbulent particle dispersion
        - Stochastic tracking

        - Particle cloud model (V5)
    - Pulverized coal and oil spray combustion submodels
- Radiation models: DTRM, P-1, Rosseland and Discrete Ordinates (V5)
- Turbulence models: *k-ε*, RNG *k-ε*, RSM, Realizable *k-ε* (V5) and LES (V5)
- Pollutant models: NO_X with reburn chemistry (V5) and soot [15]

4.2.4. Modeling chemical kinetics in combustion

- Challenging
    - Most practical combustion processes are turbulent
    - Rate expressions are highly nonlinear; turbulence-chemistry interactions are important
    - Realistic chemical mechanisms have tens of species, hundreds of reactions and stiff kinetics (widely disparate time scales)
- Practical approaches
    - Reduced chemical mechanisms
        - Finite rate combustion model
    - Decouple reaction chemistry from turbulent flow and mixing
        - Mixture fraction approaches
            - Equilibrium chemistry PDF model
            - Laminar flamelet
        - Progress variable
            - Zimont model [15]

4.3. Physical Models For Flow And Heat Transfer In Fluent

4.3.1. Mass conservation equation

The equation for conservation of mass, or continuity equation, can be written as fallows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = S_m \tag{4.1}$$

Equation 4.1 is the general form of the mass conservation and is valid for incompressible as well as compressible flows. The source S_m is the mass added to the continues phase from the dispersed second phase (e.g., due to vaporization of liquid droplets) and any user-defined sources.

For 2D axisymmetric geometries, the continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial r}(\rho v) + \frac{\rho v}{r} = S_m \tag{4.2}$$

where x is the axial coordinate, r is the radial coordinate, u is the axial velocity, and v is the radial velocity.[16]

4.3.2. Momentum conservation equation

Conservation of momentum in the i th direction in an inertial (non accelerating) reference frame is described by

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i \tag{4.3}$$

where p is the static pressure, τ_{ij} is the stress tensor (described below), and ρg_i and F_i are the gravitational body force and external body forces (e.g., that arise from interaction with the dispersed phase) in the i direction, respectively. F_i also contains other model-dependent source terms such as centrifugal and Coriolis forces and porous-media and user-defined sources.

The stress tensor τ_{ij} is given by

$$\tau_{ij} = \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial u_l}{\partial x_l} \delta_{ij} \tag{4.4}$$

where μ is the molecular viscosity and the second term on the right hand side is the effect of volume dilation.

For 2D axisymmetric geometries, axial and radial momentum conservation equations are given by

$$\frac{\partial}{\partial t}(\rho u) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho uu) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho vu) = -\frac{\partial p}{\partial x} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu \left(2\frac{\partial u}{\partial x} - \frac{2}{3}(\nabla . \vec{v}) \right) \right]$$

$$+ \frac{1}{r}\frac{\partial}{\partial r}\left[r\mu \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \right] + F_x \tag{4.5}$$

and

$$\frac{\partial}{\partial t}(\rho v) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho uv) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho vv) = -\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial r}\right)\right]$$

$$+\frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(2\frac{\partial v}{\partial r}-\frac{2}{3}(\nabla.\underset{v}{\rho})\right)\right]$$

$$-2\mu\frac{v}{r^2}+\frac{2}{3}\frac{\mu}{r}(\nabla.\underset{v}{\rho})+\rho\frac{w^2}{r}+F_r \qquad (4.6)$$

where

$$\nabla.\underset{v}{\rho}=\frac{\partial u}{\partial x}+\frac{\partial v}{\partial r}+\frac{v}{r} \qquad (4.7)$$

and w is the swirl velocity.[16]

4.3.3. Turbulence model

4.3.3.1. Standard $k-\varepsilon$ model

The standard $k-\varepsilon$ model is a semi-empirical model. The model equations are derived from the Reynolds-Averaged Navier-Stokes (RANS) equations. Its derivation is based on the assumption that the flow is fully turbulent, and the effects of molecular viscosity are negligible. The standard $k-\varepsilon$ model is therefore valid only for fully turbulent flows.[16]

4.3.3.2. Reynolds (ensemble) averaging

The standard $k-\varepsilon$ model in Fluent, like other conventional turbulence models, is based on Reynolds averages of the governing equations. In the Reynolds averaging, all the solution variables in the original Navier-Stokes equations are decomposed into the mean (ensemble-averaged or time-averaged) and fluctuating components. For velocity components:

$$u_i = \bar{u}_i + u_i' \tag{4.8}$$

where $\bar{u}_i$ and u_i' are the mean and instantaneous velocity components (i=1,2,3).

Likewise, for pressure and other scalars:

$$\phi = \bar{\phi} + \phi' \tag{4.9}$$

where ϕ denotes general scalars (pressure, enthalpy, species-concentration, etc.)

Substituting the expressions of this form for the flow variables into the instantaneous continuity and momentum equations and taking a time (or ensemble) average (and dropping the overbar on the mean velocity, $\bar{u}$) yields the ensemble-averaged momentum equations. They can be written in Cartesian tensor form as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0 \tag{4.10}$$

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \left(\frac{2}{3}\mu\frac{\partial u_l}{\partial x_l}\right)\right] - \frac{\partial p}{\partial x_i}$$

$$+ \frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right) \tag{4.11}$$

Equations 4.10 and 4.11 are called ‘’Reynolds-Averaged’’ Navier-Stokes (RANS) equations, and have the same forms as the instantaneous Navier-Stokes equations, with the velocities and other solution variables now representing ensemble-averaged (or time-averaged) values. In the RANS equations, effects of turbulence are represented by the ‘’Reynolds stresses’’,

- $\rho\overline{u_i' u_j'}$ **.** These Reynolds stresses need to be modeled in order to close equation 4.11.

Equations 4.10 and 4.11 can be applied to density-varying flows.[16]

4.3.3.3. Equations for the standard $k-\varepsilon$ model

In the standard $k-\varepsilon$ model, Reynolds stresses in Equation 4.11 are modeled using the Boussinesq hypothesis:

$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\left(\rho k+\mu_t\frac{\partial u_i}{\partial x_i}\right)\delta_{ij} \tag{4.12}$$

The ‘’eddy’’’ or turbulent viscosity, μ_t, is computed using turbulent kinetic energy (k) and its rate of dissipation (ε) from

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{4.13}$$

Turbulent kinetic energy (k) and its rate of dissipation (ε) in Equation 8.3-6 are obtained from the solutions of their ‘’modeled’’ transport equations

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho u_i k)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right]+G_k+G_b-\rho\varepsilon \tag{4.14}$$

and

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho u_i\varepsilon)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_i}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\{G_k+(1-C_{3\varepsilon})G_b\}-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}$$

(4.15)

where G_k is the generation of k due to the turbulent stress, and is given by

$$G_k=-\rho\overline{u_i'u_j'}\frac{\partial u_j}{\partial x_i} \tag{4.16}$$

and G_b is the generation of k due to buoyancy:

$$G_b=\beta g_i\frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial T}{\partial x_i} \tag{4.11}$$

where Pr_t is the turbulent Prandtl number for temperature or enthalpy, and β is the coefficient of thermal expansion:

$$\beta=-\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_p \tag{4.12}$$

For ideal gases, Equation 4.11 reduces to

$$G_b=-g_i\frac{\mu_t}{\rho\,\mathrm{Pr}_t}\frac{\partial\rho}{\partial x_i} \tag{4.13}$$

the model constants $C_{1\varepsilon}, C_{2\varepsilon}, C_{\mu}, \sigma_k, \sigma_\varepsilon$ have the fallowing default values:

$C_{1\varepsilon}$=1.44, $C_{2\varepsilon}$=1.92, C_{μ}=0.09, σ_k=1.0, σ_ε=1.3, Pr_t=0.85

These default values have been determined from experiments with air and water for fundamental turbulent shear flows including homogeneous shear flows and isotropic grid turbulence. They have been found to work fairly well for a wide range of wall-bounded and free shear flows.

Although the default values of the model constants are the standard ones most widely accepted, they can be changed (if needed) in the Viscous Model panel.[16]

4.3.3.4. Heat and mass transfer modeling in the standard $k-\varepsilon$ model

In Fluent, turbulent heat transport is modeled using the concept of Reynolds' analogy to turbulent momentum transfer. The ''modeled'' energy equation is thus given by

$$\frac{\partial}{\partial t}(\rho h)+\frac{\partial}{\partial x_i}(\rho u_i h)=\frac{\partial}{\partial x_i}\left[\left(k+\frac{\mu_t}{\mathrm{Pr}_t}\right)\frac{\partial T}{\partial x_i}\right]+\frac{D_p}{D_t}+(\tau_{ik})_{eff}\frac{\partial u_i}{\partial x_k}+S_h \qquad (4.14)$$

where h is the sensible enthalpy, k is the molecular conductivity, τ_{ik} is the deviatoric stress tensor, and Pr_t is the turbulent Prandtl number for temperature or enthalpy. The turbulence heat transfer is thus dictated by the turbulent viscosity (μ_t) and turbulent Prandtl number (Pr_t). In Fluent, the default value of the turbulent Prandtl number is 0.85. The value can be changed in the Viscous Model panel.

Turbulent mass transfer is treated similarly using the Reynolds analogy with the momentum transfer. The default turbulent Schmidt number is 0.7. This default value can also be changed in the Viscous Model panel.[16]

4.3.3.5. Compressibility effects in the standard $k-\varepsilon$ model

For high-Mach-number flows, compressibility effects turbulence through so-called ''dilatation dissipation'', which is normally neglected in the modeling of incompressible flows. Neglecting the dilatation dissipation fails to predict the observed decrease in spreading rate with increasing Mach number for compressible

mixing and other free shear layers. In Fluent, the dilatation dissipation is modeled following Sarkar's proposal. In Sarkar's model, the k equation is given by

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho u_i k)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right]+G_k+G_b-\rho\varepsilon\left(1+2M_t^2\right) \tag{4.15}$$

The turbulent Mach number, M_t, is defined as

$$M_t=\sqrt{\frac{k}{a^2}} \tag{4.16}$$

where $a\left(\equiv\sqrt{\gamma RT}\right)$ is the speed of sound.

This compressibility modification always takes effect when the compressible form of the ideal gas law is used.[16]

4.3.4. The energy equation

The energy equation can be written in terms of sensible enthalpy h as

$$\frac{\partial}{\partial t}(\rho h)+\frac{\partial}{\partial x_i}(\rho u_i h)=\frac{\partial}{\partial x_i}(k+k_t)\frac{\partial T}{\partial x_i}-\frac{\partial}{\partial x_i}\sum_{j'}h_{j'}J_{j'}+\frac{D_p}{D_t}+\left(\tau_{ik}\right)_{eff}\frac{\partial u_i}{\partial x_k}+S_h \tag{4.17}$$

where k is the molecular conductivity, k_t is the conductivity due to turbulent transport $\left(k_t=c_p\mu_t/\mathrm{Pr}_t\right)$, $J_{j'}$ is the diffusion flux of the species j', and the source term S_h includes heat of chemical reaction, any inter-phase exchange of heat, and any other defined volumetric heat sources.

Sensible enthalpy h is defined as

$$h = \sum_{j'} m_{j'} h_{j'} \tag{4.18}$$

where $m_{j'}$ is the mass fraction of species j' and

$$h_{j'} = \int_{T_{ref}}^{T} c_{p,j'} dT \tag{4.19}$$

where T_{ref} is 298.15 K.

Fluent solves equation 4.17 using temperature as the dependent variable. The left-hand side of equation 4.17 is transformed to a temperature form by using equations 4.18 and 4.19. When the non-adiabatic PDF combustion model is enabled, Fluent solves a reduced form of equation 4.17, under the assumption of Lewis number = 1:

$$\frac{\partial}{\partial t}(\rho H) + \frac{\partial}{\partial x_i}(\rho u_{iH}) = \frac{\partial}{\partial x_i}\left(\frac{k_t}{c_p}\frac{\partial H}{\partial x_i}\right) + \tau_{ik}\frac{\partial u_i}{\partial x_k} + S_h \tag{4.20}$$

The enthalpy H is defined as

$$H = \sum_{j'} m_{j'} H_{j'} \tag{4.21}$$

where $m_{j'}$ is the mass fraction of species j' and

$$H_{j'} = \int_{T_{ref,j'}}^{T} c_{p,j'} dT + h_{j'}^{0}\left(T_{ref,j'}\right) \tag{4.22}$$

$h^0_{j'}(T_{ref,j'})$ is the formation enthalpy of species j' at the reference temperature $T_{ref,j'}$ [16]

4.3.5. Inclusion of the species diffusion term

Equation 4.17 includes the effect of enthalpy transport due to species diffusion;

$$\frac{\partial}{\partial x_i}\sum_{j'} h_{j'} J_{j'} \tag{4.23}$$

which contributes to the energy balance, especially for the case of Lewis numbers far from unity. This term is included in Fluent's energy equation by default.

When the non-adiabatic PDF combustion model is being used, this term is not included, under the assumption that the Lewis number is unity.[16]

4.3.6. Energy sources due to the reaction

Sources of energy, S_h, in equation 8.4-1 include the source of energy due to chemical reaction:

$$S_{h,reaction} = \sum_{j'}\left[\frac{h^0_{j'}}{M_{j'}} + \int_{Tref,j'}^{T_{ref}} c_{p,j'}\,dT\right] R_{j'} \tag{4.24}$$

where $h^0_{j'}$ is the enthalpy of formation of species j' and $R_{j'}$ is the volumetric rate of creation of species j'.

In the energy equation used for non-adiabatic PDF combustion (4.20), the heat of formation is included in the definition of enthalpy (4.22), so reaction sources of energy are not included in S_h.[16]

4.3.7. Energy equation in conductive solids

In conducting solid regions, Fluent solves a simple conduction equation that includes the heat flux due to conduction and volumetric heat sources within the solid:

$$\frac{\partial}{\partial t}\rho h = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \dot{q}''' \qquad (4.25)$$

where ρ is density, h is sensible enthalpy ($\int_{T_{ref}}^{T} c_p dT$) , k is conductivity, T is temperature, $\dot{q}'''$ is volumetric heat source.

Equation 4.25 is solved simultaneously with the energy transport equation,4.17, in the flow regions to yield a fully coupled conduction/convection heat transfer prediction.[16]

4.4. Experimental Approach

The test installation compose from these

Burner, radiant pipes, natural gas depot, depot-burner connection, regulator, manometers, fitting staff to the wall, exhaust fan, gas emission analyzer, thermo-staff in order to measure pipe temperature. [2]

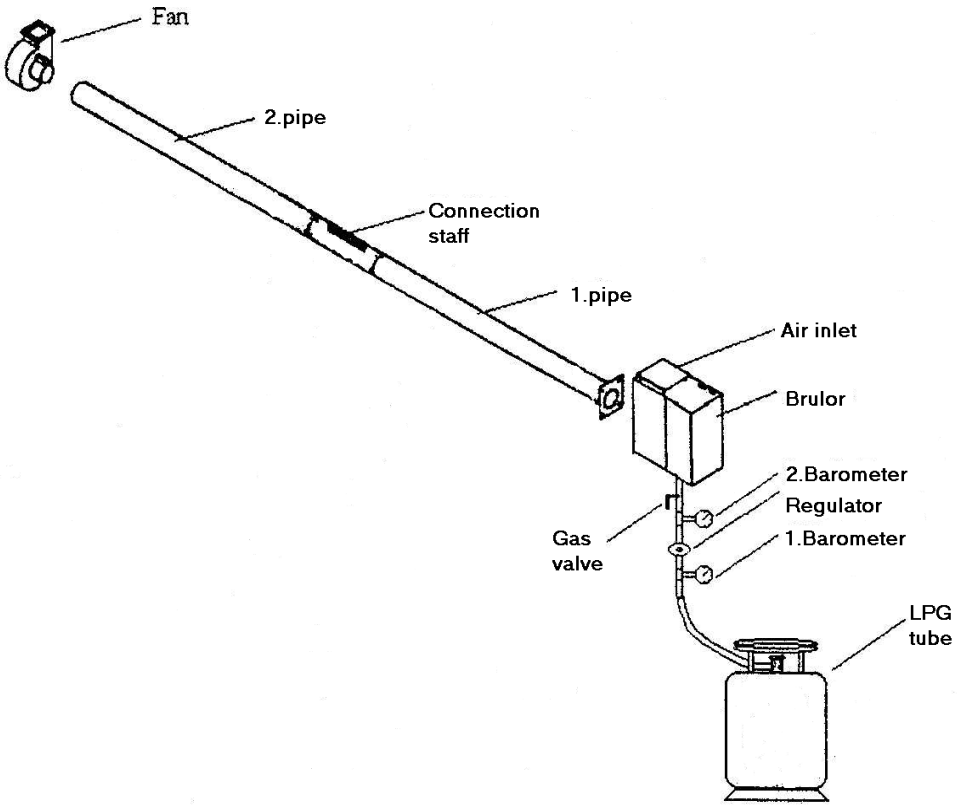


Figure 4.2. Test Installation

4.4.1. Radiant system

The radiant system is ‘’Blackheat’’ marked , which has four main component: Burner, radiant pipe, reflector and vacuum pump (exhaust fan). But in the test installation there is no reflector, and the vacuum pump is another marked. The gas burned by burner, circulated and get off by the exhaust fan. The circulated gas through the pipe, leaves its heat to the pipe and surface temperature of the pipe reaches to 350 – 400 °C immediately. The beams from the pipe turn to heat as soon as reaches to the substances. Firstly substances heat up, and then heat is convected to the air from surfaces of these substances. So that, floor level is always warmer than high levels. In figure 4.3 test installation photo is shown. [2]

Figure 4.3. Photo of the Test Installation

4.4.2. Burner

The technical properties of the burner – Blackheat, 15 kW, BH15 ST code – are given in the fallowing table.

Table 4.1. Technical Properties of Burner

Model	BH 15 ST
Power (kW)	15
Total Pipe Length (mm)	6685
Total Weight (kg)	41
Heating Area (m^2)	20 – 160
Minimum Fitting Height (mm)	3.5
Gas Fuel	Natural Gas or LPG
Natural Gas Consumption (Nm^3/h)	1.56
LPG Consumption (kg/h)	1.15
Natural Gas Inlet Pressure (mBar)	min 15;max 50
LPG Inlet Pressure (mBar)	min 32.5;max 50
Gas Connection Staff	½'' Gear
Electricity Consumption	230 V, monophase, 1 A
Ignition	Full automatic, flame censored

According to user guide-handbook, the most efficiently working pressure is 18.4 mBar for LPG, 8.7 mBar for natural gas. [2]

The fallowing figure shows photo of the burner:

Figure 4.4. Burner

4.4.3. Radiant pipes

Radiant pipes radius are 100 mm, and formed form two piece of pipe both length is 3 m. They are very emissive steal pipes, and their interfaces and surfaces covered with aluminum. They are also noncorrosive. Pipe clips connect them, so that there is no gas leakage. While system work, the temperature of the pipes reaches to 350 – 400°C. [2]

4.4.4. Vacuum pump (exhaust fan)

Connected to the burner serially. It works with electricity coming from burner. The condenser at the electricity inlet provides electricity equilibrium. They empty the gases in the pipes, and create vacuum. This provides a move to the burned gas and easiness in transferring heat. [2]

4.4.5. LPG depot

12 kg home type gas depot was used in this application. [2]

4.4.6. Natural gas depot

The depot was 45 lt, resistant till 200 – 300 bar. Fallowing figure shows the depot.[2]

Figure 4.5. Natural Gas Depot

4.4.7. Gas analyzer

The analyzer, which was used to measure CO_2 and O_2 emissions, was ‘’Sun’’ marked and its model is MGA 1200. The ‘’Horiba’’ gas analyzer was used to measure NO and NO_x in natural gas test. CLA-220 is the model of analyzer.[2]

4.4.8. Thermo staff

A low sensitive staff was used in the test. It could measure till 600 °C. This measured the temperatures of the certain regions of the pipe.[2]

4.5. The Test and Results

First test was done with LPG, and the other two tests were done with natural gas.

After 15 min later from first ignition, the temperatures of 6 points of the pipe were measured. The distances between points were 1 m. Points are shown in the fallowing figure.

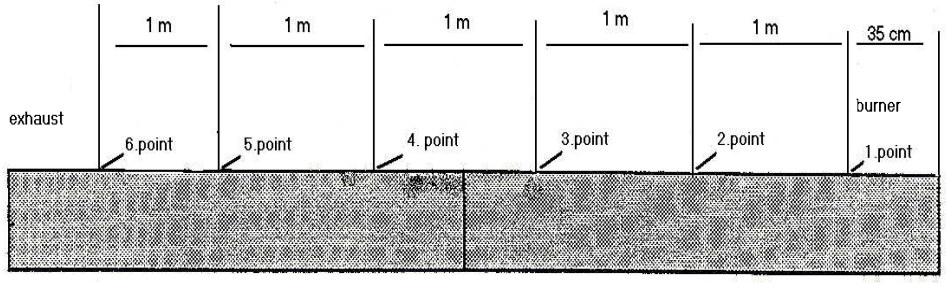


Figure 4.6. The Points on the Pipe Surface

After CO_2 and O_2 emissions become in steady state, measurement had been done. And the results are shown in the fallowing table.[2]

Table 4.2. The Results of the Test

Test	Pressure Inlet (mBar)	%vol O_2	%vol CO_2	1.point [°C]	2.point [°C]	3.point [°C]	4.point [°C]	5.point [°C]	6.point [°C]	λ
1(LPG)	2.5	18.6	1.54	255	240	215	195	180	175	9.08
2(NG)	24	18.9	0.068	200	180	165	150	140	135	10.45
3(NG)	20	19.0	0.66	200	185	170	150	145	145	11.00

4.6. Simulation Of The System

4.6.1. Creating geometry

Simplified geometry has to be created, firstly. The geometry have to be mashed and then boundaries of the system defined.

The original geometry of the burner is shown in figure 4.7. , is very complicated for first solving. So, it was simplified as figure 4.8.

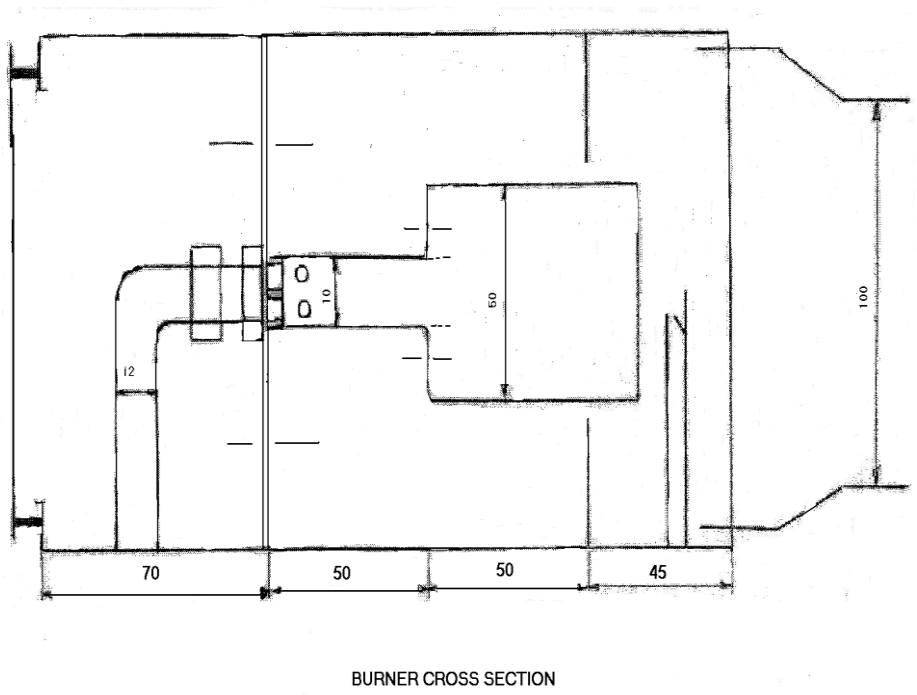


Figure 4.7. Burner Cross Section

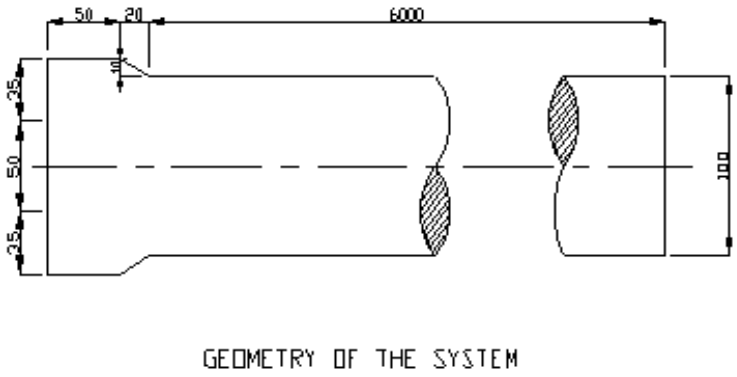


Figure 4.8. Simplified Geometry

The Grid, created in Gambit, is shown in fallowing figure.

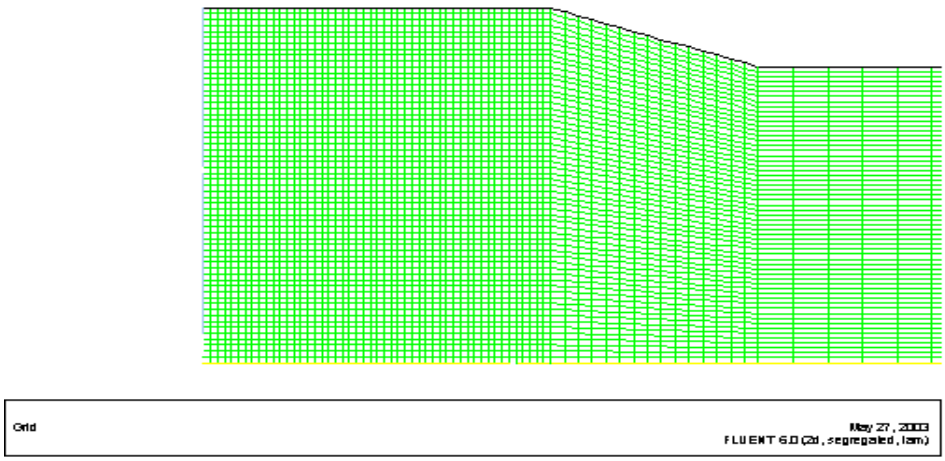


Figure 4.9. The Grid

4.6.2. Selecting combusiton model

In order to solve the problem fallowing choices have been selected.

- Diffision flame model was selected
- The domain defined was axisymetric
- K-ε standard viscous model was selected as turbulence model
- No radiation was assumed
- Species Transport model was selected as finite rate for methane-air gas mixture
- Methane-air mixture was selected as mixture materials
- Eddy-Dissipation was selected as reaction model
- Ideal gas mixing low was used for density

4.6.3. Defining the Boundary Conditions

Fallowing conditions has been accepted for this simulation.

- The symmetry was converted to the axis
- Suitable values were given for velocity magnitude, temperature, turbulence method, and species mass fractions for air, fuel inlets and pressure outlet.
- Acceptable conditions were set for the walls.
- The value of 2000 –3000 K was given for the temperature as initial condition
- Mass fraction of CH_4 was adjusted as 0.2
- The value of 0.001 was given as convergence criterion for all residuals except energy
- 10^{-6} was selected for the energy.

4.6.4. Calculating of suitable velocity

The power of the burner is 15 kw

$$\dot{Q} = \dot{m}_f \Delta h \qquad (4.26)$$

$$\dot{m}_f = 15000 / 5001600 = 2{,}9.10^{-3}\, kg/s$$

and

$$\rho_f = P / \left[(R_u / MW_{fuel}) T \right] \qquad (4.27)$$

where

P = 101325 N/m^2, R = 8315 J/kmol, MW=16 kg/kmol and T = 300 K

Then

$\rho_f = 0.65$ kg/m^3 was found.

Volumetric flow rate of fuel is

$$Q_f = m_f / \rho \qquad (4.28)$$

$Q_f = 4.5.10^{-3}$ m^3/s

since flow rate is

$$Q = A.V \qquad (4.29)$$

and the area at fuel inlet is

$A = \pi (5.10^{-3})^2$

then the fuel velocity was calculated as

$V_f = 56.6$ m/s

After a few try the most suitable value for air velocity is founded as 2.8 m/s for our geometry.

The results of the simulation for these values were given at appendix.

4.7. Evaluation Of The Simulation

The results of test and simulation are not completely the same. It may be occurred because of few reasons such as:

The geometry created in gambit is too much simply. The grid can be improved and the dense of the mesh can be increased.

The convergence criteria's for the products may be decreased between 10-100 times because in this study no products found at the exhaust. But this assumption requires long calculating time from computer.

After the suitable product values are found, the air excess coefficient can be found and compared to the experimental results.

Flame length in the pipe can be calculated dependent on the geometry of combustion chamber and properties of reactants by combustion equations of laminar diffusion flames.

Although the results do not match, the study proved that CFD helps to find an optimum combustion system faster than using pure testing alone. Very few attempts have been made to find a solution in short time.

Although modeling of the combustion is faster and cheaper than making tests, there is a disadvantages of simulation. The definitions and the roles of the options of the CFD are have to be well known because it can be seen that all changes in results are due to changes of input parameters. So that operation requires high level of skill and understanding from the operator. Good educated operators are needed in order to reach significant results. That decreases the expense of the study.

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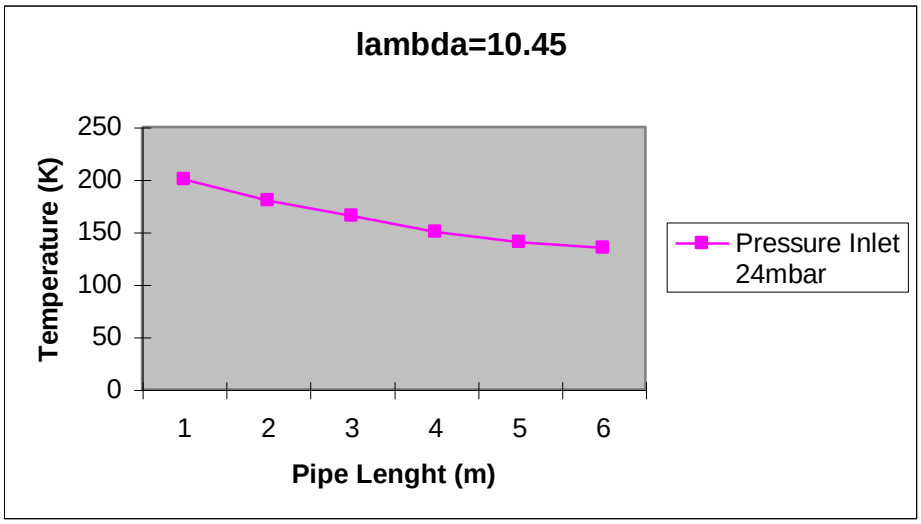
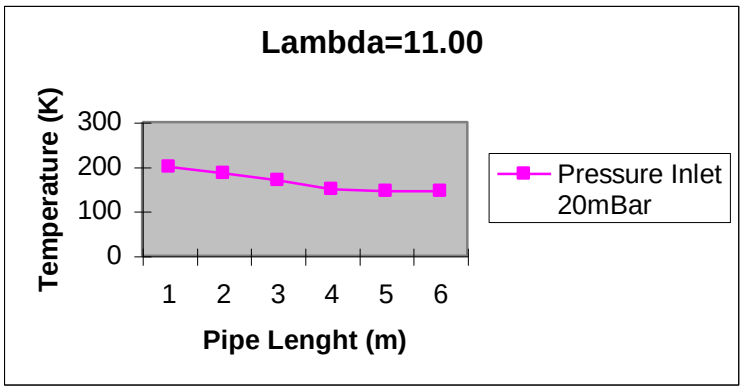
APPENDIX

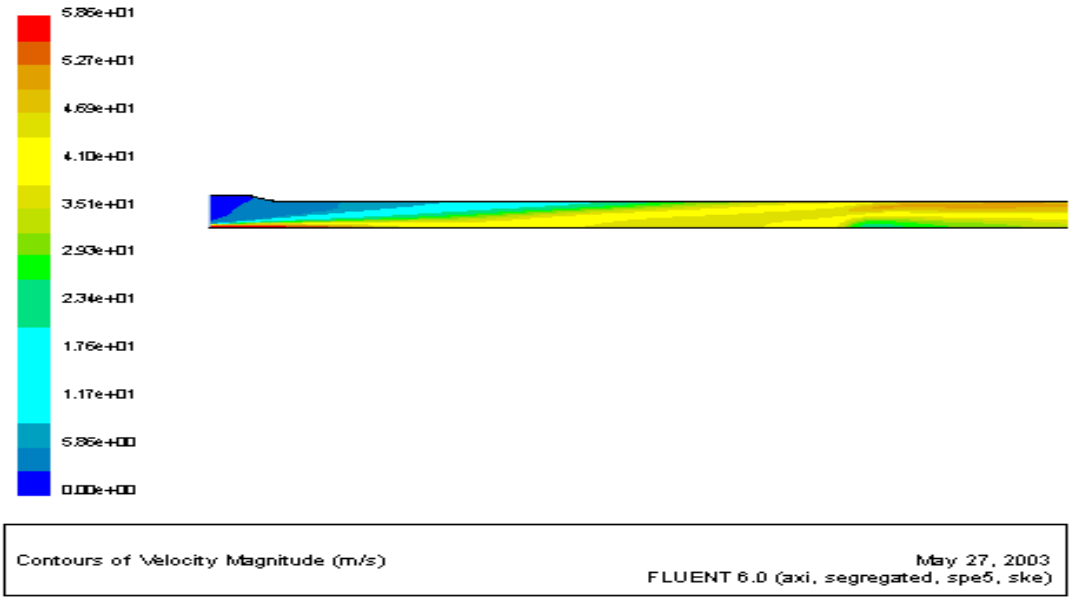
APPENDIX I	Test results for 18.9 %O2 and 0.068 % CO2 inlet as volumetrically
APPENDIX II	Test results for 19.0 %O2 and 0.66 % CO2 inlet as volumetrically
APPENDIX III	Contours of Velocity Magnitude (V_{air}=2.8 m/s, V_{fuel} = 56.6 m/s)
APPENDIX IV	Contours of Static Temperature (T_{max} = 2970 K)
APPENDIX V	Contours of Mass Fraction of CH_4
APPENDIX VI	Contours of Mass Fraction of O_2
APPENDIX VII	Mole fraction of O_2
APPENDIX VIII	Mass fraction of CH_4
APPENDIX IX	Mass fraction of CO_2
APPENDIX X	Mass fraction of H_2O
APPENDIX XI	Mass fraction of N_2



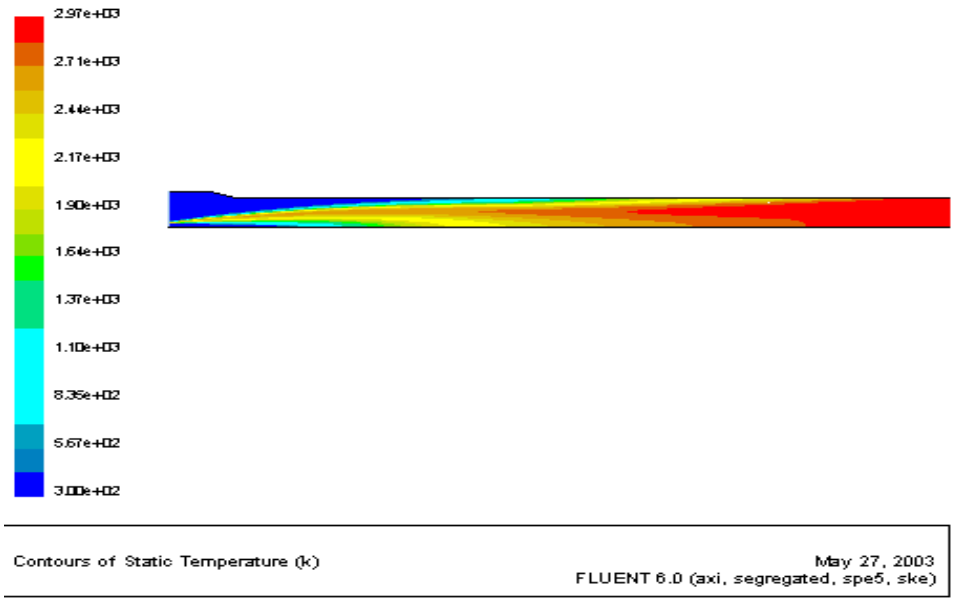
APPENDIX I - Test results for 18.9 %O_2 and 0.068 % CO_2 inlet as volumetrically



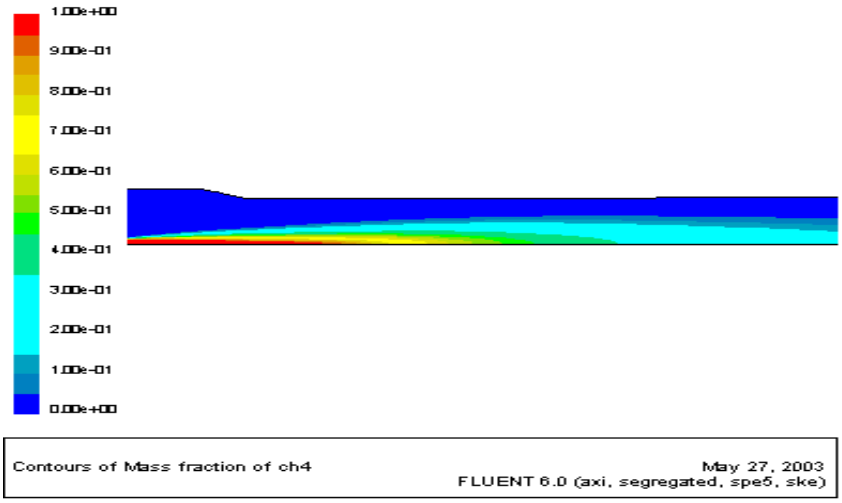
APPENDIX II - Test results for 19.0 %O_2 and 0.66 % CO_2 inlet as volumetrically



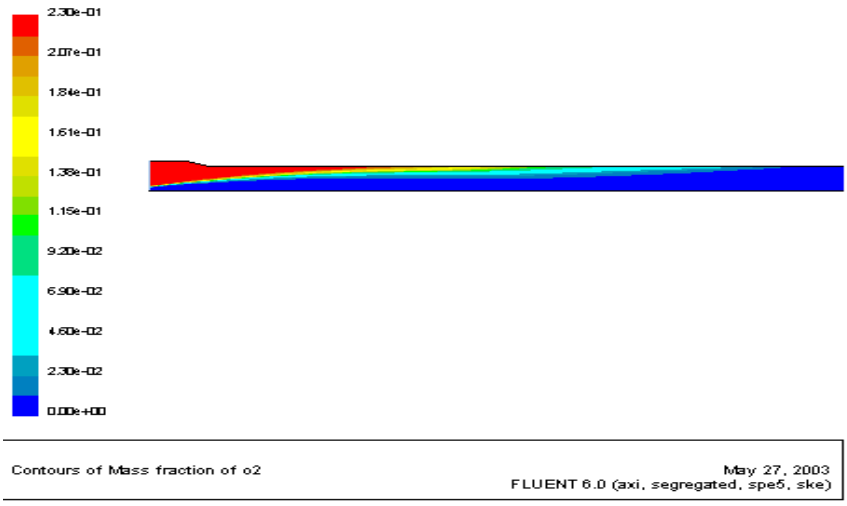
APPENDIX III - Contours of Velocity Magnitude (V_{air}=2.8 m/s, V_{fuel} = 56.6 m/s)



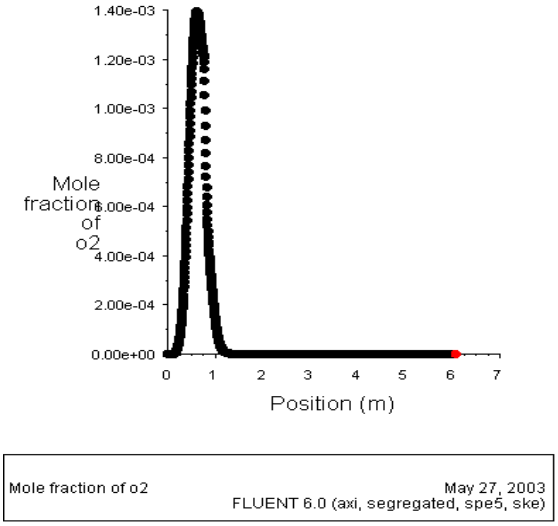
APPENDIX IV - Contours of Static Temperature (T_{max} = 2970 K)



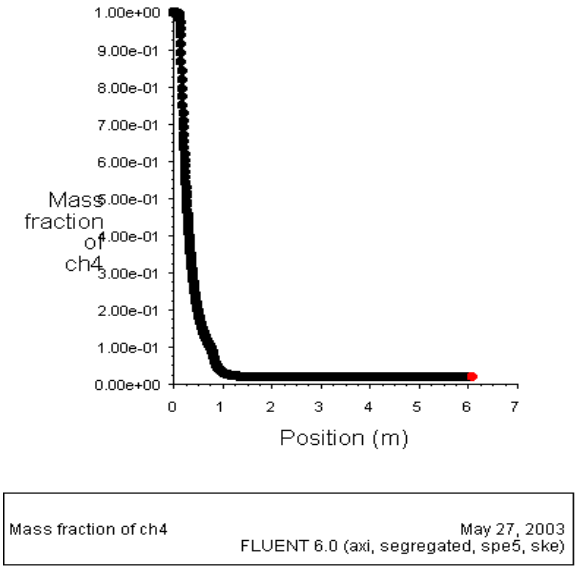
APPENDIX V - Contours of Mass Fraction of CH_4



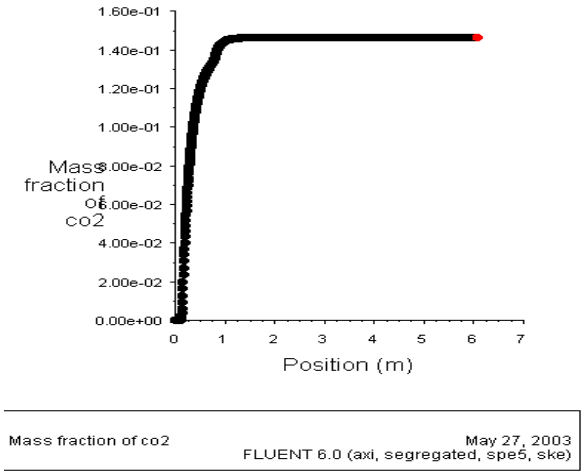
APPENDIX VI – Contours of Mass Fraction of O_2



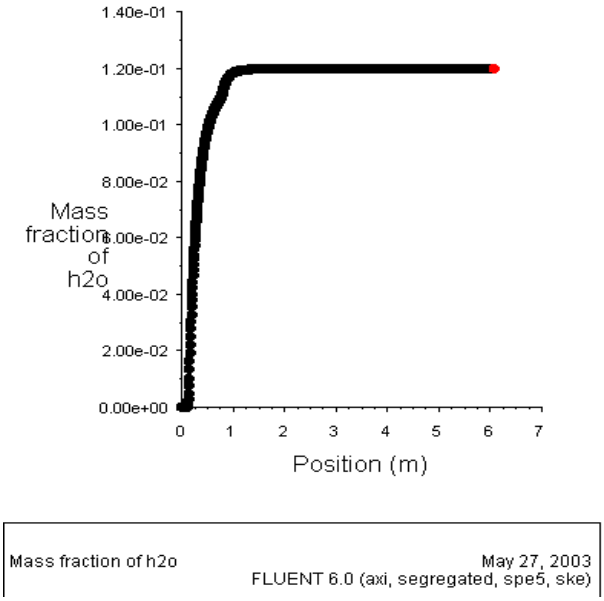
APPENDIX VII – Mole fraction of O_2



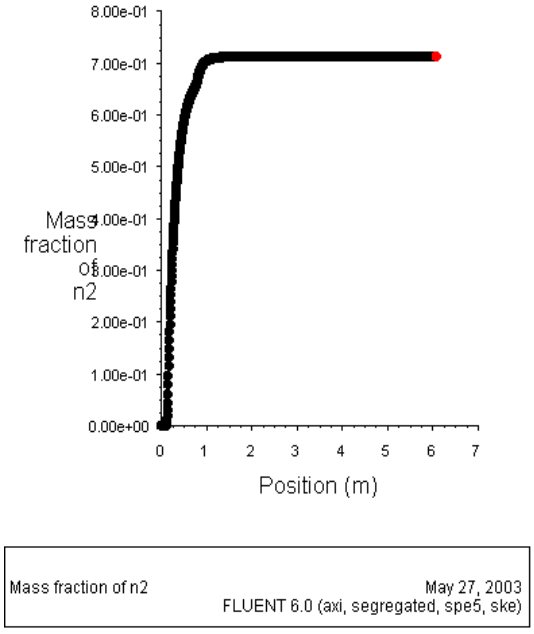
APPENDIX VIII – Mass fraction of CH_4



APPENDIX IX – Mass fraction of CO_2



APPENDIX X – Mass fraction of H_2O



APPENDIX XI- Mass fraction of N_2

ÖZGEÇMİŞ

Oğuz KURTİLİ, 06/08/1978 tarihinde Almanya'nın Hameln kentinde dünyaya geldi. 1984 yılında Türkiye'ye kesin dönüş yaptı ve aynı sene İstanbul'un Fatih semtindeki Muallim Yahya Efendi İlkokulu'nda öğretim hayatına basladı. Ortaokulu Fatih Ahmet Rasim Lisesi'nde okudu. Lise eğitimini 1995 yılında Özel Fatih Erkek Fen Lisesi'nde tamamladıktan sonra aynı sene üniversite sınavında Yıldız Teknik Üniversitesi Makine Mühendisliği bölümünü kazandi. 1999 yılında bu okuldan mezun oldu ve aynı sene İstanbul Teknik Üniversitesi Fen Bilimleri Enstitüsü'nün Makine Mühendisliği Otomotiv programına girdi. Yüksek lisans eğitiminde mühendislikte simülasyon konusuna ilgi duydu ve bu alanda bir tez çalışmasıyla 2003 yılında yüksek lisansını tamamladı.